

Free energy density for mean field perturbation of states of a one-dimensional spin chain

Dedicated to Professor Walter Thirring on his 80th birthday

Fumio Hiai¹, Milán Mosonyi², Hiromichi Ohno³ and Dénes Petz⁴

^{1,2} Graduate School of Information Sciences, Tohoku University
Aoba-ku, Sendai 980-8579, Japan

³ Graduate School of Mathematics, Kyushu University,
1-10-6 Hakozaki, Fukuoka 812-8581, Japan

⁴ Alfréd Rényi Institute of Mathematics,
H-1364 Budapest, POB 127, Hungary

Abstract

Motivated by recent developments on large deviations in states of the spin chain, we reconsider the work of Petz, Raggio and Verbeure in 1989 on the variational expression of free energy density in the presence of a mean field type perturbation. We extend their results from the product state case to the Gibbs state case in the setting of translation-invariant interactions of finite range. In the special case of a locally faithful quantum Markov state, we clarify the relation between two different kinds of free energy densities (or pressure functions).

AMS subject classification: 82B10, 82B20

Key words and phrases: free energy density, mean relative entropy, interactions, Gibbs states, KMS states, finitely correlated states, quantum Markov states, Legendre transform

¹E-mail: hiai@math.is.tohoku.ac.jp; Partially supported by Grant-in-Aid for Scientific Research (B)17340043.

²E-mail: milan.mosonyi@gmail.com; Partially supported by Grant-in-Aid for JSPS Fellows 18 · 06916.

³E-mail: ohno@math.kyushu-u.ac.jp; Partially supported by Grant-in-Aid for JSPS Fellows 19 · 2166.

⁴E-mail: petz@math.bme.hu; Partially supported by the Hungarian Research Grant OTKA T068258.

1 Introduction

The theoretical description of the statistical mechanics of quantum spin chains was the first success of the operator algebraic approach to quantum physics. A one-dimensional spin chain is described by a quasi-local C^* -algebra $\mathcal{A} := \bigotimes_{k \in \mathbb{Z}} \mathcal{A}_k$ which is the infinite tensor product of full matrix algebras $\mathcal{A}_k = M_d(\mathbb{C})$ and the limit of the local algebras $\mathcal{A}_\Lambda := \bigotimes_{k \in \Lambda} \mathcal{A}_k$, where $\Lambda \subset \mathbb{Z}$ is finite. A state φ of the spin chain is uniquely specified by its local restrictions $\varphi_\Lambda := \varphi|_{\mathcal{A}_\Lambda}$. A local state ω of \mathcal{A}_Λ can equivalently be given by its density matrix $D(\omega)$ satisfying $\omega(A) = \text{Tr } D(\omega)A$, $A \in \mathcal{A}_\Lambda$.

A translation-invariant interaction Φ of the spins determines a *local Hamiltonian*

$$H_\Lambda(\Phi) := \sum_{X \subset \Lambda} \Phi(X) \quad (1.1)$$

with corresponding *local Gibbs state*

$$D(\varphi_\Lambda^G) := \frac{e^{-H_\Lambda(\Phi)}}{\text{Tr } e^{-H_\Lambda(\Phi)}} \quad (1.2)$$

for all finite $\Lambda \subset \mathbb{Z}$. The local Gibbs state is the unique maximizer of the functional $\omega \mapsto -\omega(H_\Lambda(\Phi)) + S(\omega)$, where ω is an arbitrary state of \mathcal{A}_Λ and $S(\omega)$ is the von Neumann entropy $S(\omega) := -\text{Tr } D(\omega) \log D(\omega)$. Furthermore,

$$\log \text{Tr}_\Lambda e^{-H_\Lambda(\Phi)} = \max\{-\omega(H_\Lambda(\Phi)) + S(\omega) : \omega \text{ state of } \mathcal{A}_\Lambda\}. \quad (1.3)$$

One of the main problems in the statistical mechanics of the spin chain is the determination of the global equilibrium states of \mathcal{A} for a given interaction. When Φ is of relatively short range, it is well known [11, 22] that the variational formula (1.3) holds in the asymptotic limit:

$$P(\Phi) = \max\{-\omega(A_\Phi) + s(\omega) : \omega \text{ translation-invariant state of } \mathcal{A}\}, \quad (1.4)$$

where

$$P(\Phi) := \lim_{\Lambda \rightarrow \mathbb{Z}} \frac{1}{|\Lambda|} \log \text{Tr } e^{-H_\Lambda(\Phi)}, \quad (1.5)$$

$$s(\omega) := \lim_{\Lambda \rightarrow \mathbb{Z}} \frac{1}{|\Lambda|} S(\omega|_{\mathcal{A}_\Lambda}), \quad (1.6)$$

$$A_\Phi := \sum_{X \ni 0} \frac{\Phi(X)}{|X|} \quad (1.7)$$

are the *pressure* (or *free energy density*) of Φ , the *mean entropy* of ω and the *mean energy* of Φ , respectively. (Here note that the term “free energy” should be used with minus sign in the exact sense of physics.) Maximizers of the right-hand side of (1.4) are the equilibrium states for the interaction Φ . If Φ is of finite range, then the equilibrium state is unique.

One of the main subjects of the present paper is an extension of the free energy density (1.5) when the interaction is perturbed by a mean field term. Let γ be the right-translation automorphism of \mathcal{A} and set

$$s_n(A) := \frac{1}{n} \sum_{\Lambda + k \subset [1, n]} \gamma^k(A) \in \mathcal{A}_{[1, n]}$$

for a fixed $A \in \mathcal{A}_\Lambda^{\text{sa}}$ with a finite $\Lambda \subset \mathbb{Z}$. We will study the limit

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp(-H_{[1,n]}(\Phi) - n f(s_n(A))) , \quad (1.8)$$

where f is a real continuous function. This kind of problem was initiated by Petz, Raggio and Verbeure [33] in the particular case when there is no interaction between the spins. The motivation came from mean field models and the extension of large deviation theory for quantum chains [32]. An important tool was Størmer's quantum version of the de Finetti theorem for symmetric states. The subject was treated in details in the monograph [31] under the name "perturbational limits" by using the concept of approximately symmetric sequences [36]. Since the interaction Φ in the general situation is not invariant under the permutation of the spins, our method in the general case is the extremal decomposition theory for translation-invariant states that is standard in quantum statistical mechanics, see [10]. In the present paper we will show that the limit is expressed by a variational formula generalizing (1.4).

The limit (1.8) has a direct physical meaning in the case when $f(x) = x^2$ and $A = A_0 \in \mathcal{A}_0$. Then

$$-H_{[1,n]}(\Phi) - \frac{1}{n} \sum_{i,j=1}^n A_i A_j$$

is a mean field perturbation of the interaction Φ , where $A_j := \gamma^j(A_0)$. The limit is the free energy density for the mean field model and the variational formula has an important physical interpretation.

The limit density (1.8) can be considered in a different way as well. Given a translation-invariant state φ , we can study the limit

$$p_\varphi(A, f) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi|_{\mathcal{A}_{[1,n]}}) - n f(s_n(A))) \quad (1.9)$$

and its variational expression under the duality between the observable space \mathcal{A}^{sa} and the translation-invariant state space $\mathcal{S}_\gamma(\mathcal{A})$. In particular, when $f(x) = x$, the limit (1.9) becomes a simply perturbed free energy density function (or pressure function)

$$p_\varphi(A) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi|_{\mathcal{A}_{[1,n]}}) - n s_n(A))$$

for local observables A in \mathcal{A}^{sa} (if the limit exists). The dual function of the function $p_\varphi(A)$ is the *mean relative entropy*

$$S_M(\omega, \varphi) := \lim_{n \rightarrow \infty} \frac{1}{n} S(\omega|_{\mathcal{A}_{[1,n]}}, \varphi|_{\mathcal{A}_{[1,n]}}) \quad (1.10)$$

with respect to φ defined for $\omega \in \mathcal{S}_\gamma(\mathcal{A})$. The existence of the mean relative entropy and its properties were worked out in [18, 20, 21].

When Φ is a translation-invariant interaction of finite range and φ is the equilibrium state for Φ , the limits (1.8) and (1.9) are the same (up to an additive term $P(\Phi)$), but (1.9) can also be studied for a wider class of translation-invariant states, for example, for finitely correlated states which were introduced by Fannes, Nachtergaele and Werner [14]. A slightly different concept of quantum Markov states was formerly introduced by Accardi and Frigerio [3]. A

translation-invariant and locally faithful quantum Markov state in the sense of Accardi and Frigerio is known to be a finitely correlated state as well as the equilibrium state for a nearest-neighbor interaction [4, 30]. Remarkably, a Markovian structure similar to the special quantum Markov state just mentioned appears in the recent characterization [15, 28] of the quantum states which saturate the strong subadditivity of von Neumann entropy.

A similar but different version of the free energy density function $p_\varphi(A)$ is

$$\tilde{p}_\varphi(A) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \varphi(e^{ns_n(A)}) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \varphi \left(\exp \left(\sum_{k=1}^n \gamma^k(A) \right) \right),$$

which gives the logarithmic moment generating function for a sequence of compactly supported probability measures on the real line. Large deviations governed by this generating function have recently been studied in [29, 26, 17] for example. In fact, our first motivation of the present paper came from large deviation results in [29, 26] with respect to Gibbs-KMS states. It is not known in general for p_φ to have the interpretation as the logarithmic moment generating function as \tilde{p}_φ does. Indeed, this question is nothing more than the so-called BMV-conjecture [9]. On the other hand, since \tilde{p}_φ is not a convex function in general, it is impossible for \tilde{p}_φ to enjoy such a variational expression as p_φ does.

The paper is organized as follows. Section 2 is a preliminary on translation-invariant interactions and Gibbs-KMS equilibrium states of the one-dimensional spin chain. In Section 3 the existence of the functional free energy density (1.9) and its variational expression are obtained when φ is the Gibbs state for a translation-invariant interaction of finite range. In Section 4 the existence of the density $p_\varphi(A)$ is proven for a general finitely correlated state φ , and the exact relation between the functionals p_φ and \tilde{p}_φ introduced above is clarified in the special case when φ is a locally faithful quantum Markov state. Section 5 is a brief guide to how our results for a Gibbs state φ can be extended to the case of arbitrary dimension.

2 Preliminaries

A one-dimensional spin chain is described by the infinite tensor product C^* -algebra $\mathcal{A} := \bigotimes_{k \in \mathbb{Z}} \mathcal{A}_k$ of full matrix algebras $\mathcal{A}_k := M_d(\mathbb{C})$ over \mathbb{Z} . The right-translation automorphism of \mathcal{A} is denoted by γ . We denote by $\mathcal{S}_\gamma(\mathcal{A})$ the set of all γ -invariant states of \mathcal{A} . The C^* -subalgebra of \mathcal{A} corresponding to a subset X of \mathbb{Z} is $\mathcal{A}_X := \bigotimes_{k \in X} \mathcal{A}_k$ with convention $\mathcal{A}_\emptyset := \mathbb{C}\mathbf{1}$, where $\mathbf{1}$ is the identity of \mathcal{A} . If $X \subset Y \subset \mathbb{Z}$, then $\mathcal{A}_X \subset \mathcal{A}_Y$ by a natural inclusion. The local algebra is the dense $*$ -subalgebra $\mathcal{A}_{\text{loc}} := \bigcup_{n=1}^{\infty} \mathcal{A}_{[-n, n]}$ of \mathcal{A} . The self-adjoint parts of \mathcal{A}_{loc} and \mathcal{A} are denoted by $\mathcal{A}_{\text{loc}}^{\text{sa}}$ and \mathcal{A}^{sa} , respectively. The usual trace on \mathcal{A}_X for each finite $X \subset \mathbb{Z}$ is denoted by Tr without referring to X since it causes no confusion.

An interaction Φ in \mathcal{A} is a mapping from the nonempty finite subsets of \mathbb{Z} into \mathcal{A} such that $\Phi(X) = \Phi(X)^* \in \mathcal{A}_X$ for each finite $X \subset \mathbb{Z}$. Given an interaction Φ and a finite subset $\Lambda \subset \mathbb{Z}$, we have the local Hamiltonian $H_\Lambda(\Phi)$ given in (1.1) and the *surface energy* $W_\Lambda(\Phi)$

$$W_\Lambda(\Phi) := \sum \{ \Phi(X) : X \cap \Lambda \neq \emptyset, X \cap \Lambda^c \neq \emptyset \}$$

whenever the sum converges in norm. We always assume that Φ is γ -invariant, i.e., $\gamma(\Phi(X)) = \Phi(X+1)$ for every finite $X \subset \mathbb{Z}$, where $X+1 := \{k+1 : k \in X\}$. We denote by $\mathcal{B}_0(\mathcal{A})$ the set

of all γ -invariant interactions Φ in \mathcal{A} such that

$$\|\Phi\|_0 := \sum_{X \ni 0} \|\Phi(X)\| + \sup_{n \geq 1} \|W_{[1,n]}(\Phi)\| < +\infty.$$

It is easy to see that $\mathcal{B}_0(\mathcal{A})$ is a real Banach space with the usual linear operations and the norm $\|\Phi\|_0$. Associated with $\Phi \in \mathcal{B}_0(\mathcal{A})$ we have a strongly continuous one-parameter automorphism group α^Φ of \mathcal{A} given by

$$\alpha_t^\Phi(A) = \lim_{m \rightarrow -\infty, n \rightarrow \infty} e^{itH_{[m,n]}(\Phi)} A e^{-itH_{[m,n]}(\Phi)} \quad (A \in \mathcal{A}).$$

Then it is known [6, 24] that there exists a unique α^Φ -KMS state (at $\beta = -1$) φ of \mathcal{A} , which is automatically faithful and ergodic (i.e., an extremal point of $\mathcal{S}_\gamma(\mathcal{A})$). The KMS state φ is characterized by the Gibbs condition and so it is also called the (global) *Gibbs state* for Φ . The state φ is also characterized by the *variational principle* $s(\varphi) = \varphi(A_\Phi) + P(\Phi)$, the equality case of the expression (1.4), where $P(\Phi)$, $s(\varphi)$ and A_Φ are given in (1.5)–(1.7). See [11, 22] for details on these equivalent characterizations of equilibrium states.

In the rest of this section, assume that Φ is a γ -invariant interaction of finite range, i.e., there is an $N_0 \in \mathbb{N}$ such that $\Phi(X) = 0$ whenever the diameter of X is greater than N_0 . Of course, $\Phi \in \mathcal{B}_0(\mathcal{A})$. Let φ be the α^Φ -KMS state (at $\beta = -1$) of \mathcal{A} . The next lemma will play an essential role in our discussions below; the proof can be found in [5, 7, 8].

Lemma 2.1. *There is a constant $\lambda \geq 1$ (independent of n) such that*

$$\lambda^{-1} \varphi_n \leq \varphi_n^G \leq \lambda \varphi_n$$

for all $n \in \mathbb{N}$, where φ_n^G is the local Gibbs state (1.2) with $\Lambda = [1, n]$.

For $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ and $\Psi \in \mathcal{B}_0(\mathcal{A})$ we write for short ω_n and $H_n(\Psi)$ for $\omega|_{\mathcal{A}_{[1,n]}}$ and $H_{[1,n]}(\Psi)$, respectively. Lemma 2.1 gives

$$\left| \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi_n) - H_n(\Psi)) - \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi_n^G) - H_n(\Psi)) \right| \leq \frac{\log \lambda}{n}.$$

Since

$$\text{Tr} \exp(\log D(\varphi_n^G) - H_n(\Psi)) = \frac{\text{Tr} e^{-H_n(\Phi + \Psi)}}{\text{Tr} e^{-H_n(\Phi)}},$$

we have

Lemma 2.2. *For every $\Psi \in \mathcal{B}_0(\mathcal{A})$ the limit*

$$P_\varphi(\Psi) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi_n) - H_n(\Psi))$$

exists and

$$P_\varphi(\Psi) = P(\Phi + \Psi) - P(\Phi).$$

For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ the mean relative entropy (1.10) exists and

$$S_M(\omega, \varphi) = \lim_{n \rightarrow \infty} \frac{1}{n} S(\omega_n, \varphi_n) = \lim_{n \rightarrow \infty} \frac{1}{n} S(\omega_n, \varphi_n^G), \quad (2.1)$$

see [20, p. 710]. In fact, since

$$S(\omega_n, \varphi_n^G) = -S(\omega_n) + \omega(H_n(\Phi)) + \log \text{Tr } e^{-H_n(\Phi)}$$

and

$$\lim_{n \rightarrow \infty} \frac{\omega(H_n(\Phi))}{n} = \omega(A_\Phi),$$

we have

Lemma 2.3. *For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,*

$$S_M(\omega, \varphi) = -s(\omega) + \omega(A_\Phi) + P(\Phi).$$

Hence, the function $\omega \mapsto S_M(\omega, \varphi)$ is affine and lower semicontinuous in the weak topology on $\mathcal{S}_\gamma(\mathcal{A})$.*

Theorem 2.4.

(a) *For every $\Psi \in \mathcal{B}_0(\mathcal{A})$,*

$$P_\varphi(\Psi) = \max\{-\omega(A_\Psi) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}.$$

(b) *For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,*

$$S_M(\omega, \varphi) = \sup\{-\omega(A_\Psi) - P_\varphi(\Psi) : \Psi \in \mathcal{B}_0(\mathcal{A})\}.$$

(c) *The function P_φ on $\mathcal{B}_0(\mathcal{A})$ is Gâteaux-differentiable at any $\Psi \in \mathcal{B}_0(\mathcal{A})$, i.e., the limit*

$$\partial(P_\varphi)_\Psi(\Psi') := \lim_{t \rightarrow 0} \frac{P_\varphi(\Psi + t\Psi') - P_\varphi(\Psi)}{t}$$

exists for every $\Psi' \in \mathcal{B}_0(\mathcal{A})$. Moreover, when φ^Ψ is the unique $\alpha^{\Phi+\Psi}$ -KMS state,

$$\partial(P_\varphi)_\Psi(\Psi') = -\varphi^\Psi(A_{\Psi'}).$$

Proof. The variational expressions in (a) and (b) are just rewriting of (1.4) and

$$s(\omega) = \inf\{\omega(A_\Psi) + P(\Psi) : \Psi \in \mathcal{B}_0(\mathcal{A})\}$$

thanks to Lemmas 2.2 and 2.3 (see [22, §II.3] for the above expression of $s(\omega)$ complementary to (1.4)). Note also that the maximum in (a) is attained by the unique Gibbs state for $\Phi + \Psi$.

The differentiability of P_φ in (c) was essentially shown in [26, Corollary 3.5]; we give the proof for completeness. Let $\mathcal{B}_0(\mathcal{A})^*$ be the dual Banach space of $\mathcal{B}_0(\mathcal{A})$. For each $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ define $f_\omega \in \mathcal{B}_0(\mathcal{A})^*$ by $f_\omega(\Psi) := -\omega(A_\Psi)$. Then $\omega \mapsto f_\omega$ is an injective and continuous (in the weak* topologies) affine map [22, Lemma II.1.1]; hence $\Gamma := \{f_\omega : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}$ is a weak* compact convex subset of $\mathcal{B}_0(\mathcal{A})^*$ and

$$F(f) := \begin{cases} S_M(\omega, \varphi) & \text{if } f = f_\omega \text{ with } \omega \in \mathcal{S}_\gamma(\mathcal{A}), \\ +\infty & \text{otherwise} \end{cases}$$

is a well-defined function on $\mathcal{B}_0(\mathcal{A})^*$ which is convex and weakly* lower semicontinuous. The assertion (a) means that P_φ is the conjugate function of F , which in turn implies that the conjugate function of P_φ on $\mathcal{B}_0(\mathcal{A})$ is F . By the general theory of conjugate functions (see [13, Proposition I.5.3] for example), P_φ is Gâteaux-differentiable at $\Psi \in \mathcal{B}_0(\mathcal{A})$ if and only if there is a unique $f \in \mathcal{B}_0(\mathcal{A})^*$ such that $(P_\varphi)^*(f) = f(\Psi) - P_\varphi(\Psi)$, that is, there is a unique $\varphi^\Psi \in \mathcal{S}_\gamma(\mathcal{A})$ such that

$$S_M(\varphi^\Psi, \varphi) = -\varphi^\Psi(A_\Psi) - P_\varphi(\Psi). \quad (2.2)$$

By Lemmas 2.2 and 2.3 the above equality is equivalent to the variational principle

$$s(\varphi^\Psi) = \varphi^\Psi(A_{\Phi+\Psi}) + P(\Phi + \Psi),$$

which is equivalent to φ^Ψ being the $\alpha^{\Phi+\Psi}$ -KMS state. Hence the differentiability assertion of P_φ follows. Moreover, by (a) we get

$$P_\varphi(\Psi + t\Psi') \geq -\varphi^\Psi(A_{\Psi+t\Psi'}) - S_M(\omega, \varphi)$$

for any $\Psi' \in \mathcal{B}_0(\mathcal{A})$ and $t \in \mathbb{R}$. This together with equality (2.2) for $t = 0$ gives the formula $\partial(P_\varphi)_\Psi(\Psi') = -\varphi^\Psi(A_{\Psi'})$. \square

Corollary 2.5.

(1) For every $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ so that $A \in \mathcal{A}_\Lambda^{\text{sa}}$ with a finite $\Lambda \subset \mathbb{Z}$, the free energy density

$$p_\varphi(A) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp \left(\log D(\varphi_n) - \sum_{\Lambda+k \subset [1,n]} \gamma^k(A) \right) \quad (2.3)$$

exists (independently of the choice of Λ).

(2) The function p_φ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ is Gâteaux-differentiable at any $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ in the sense that the limit

$$\lim_{t \rightarrow 0} \frac{p_\varphi(A + tB) - p_\varphi(A)}{t}$$

exists for every $B \in \mathcal{A}_{\text{loc}}^{\text{sa}}$. In particular, the function $t \in \mathbb{R} \mapsto p_\varphi(tA)$ is differentiable for every $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$.

(3) The above function p_φ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ uniquely extends to a function (denoted by the same p_φ) on \mathcal{A}^{sa} which is convex and Lipschitz continuous with

$$|p_\varphi(A) - p_\varphi(B)| \leq \|A - B\|, \quad A, B \in \mathcal{A}^{\text{sa}}.$$

(4) For every $A \in \mathcal{A}^{\text{sa}}$,

$$p_\varphi(A) = \max\{-\omega(A) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}.$$

(5) For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,

$$\begin{aligned} S_M(\omega, \varphi) &= \sup\{-\omega(A) - p_\varphi(A) : A \in \mathcal{A}_{\text{loc}}^{\text{sa}}\} \\ &= \sup\{-\omega(A) - p_\varphi(A) : A \in \mathcal{A}^{\text{sa}}\}. \end{aligned}$$

Proof. To show (1), we may assume $A \in \mathcal{A}_{[1, \ell(A)]}^{\text{sa}}$ with some $\ell(A) \in \mathbb{N}$, and set a γ -invariant interaction Ψ_A of finite range (hence $\Psi_A \in \mathcal{B}_0(\mathcal{A})$) by

$$\Psi_A(X) := \begin{cases} \gamma^k(A) & \text{if } X = [k+1, k+\ell(A)], k \in \mathbb{Z}, \\ 0 & \text{otherwise.} \end{cases}$$

Since $\sum_{k=0}^{n-\ell(A)} \gamma^k(A) = H_n(\Psi_A)$, the limit (2.3) exists by Lemma 2.2 and its independence of the choice of Λ is obvious. The differentiability in (2) immediately follows from Theorem 2.4 (c). (In fact, the derivative of p_φ at A is $\partial(p_\varphi)_A(B) = -\varphi^A(B)$ for every $B \in \mathcal{A}_{\text{loc}}^{\text{sa}}$, where φ^A is the unique $\alpha^{\Phi+\Psi_A}$ -KMS state.) Moreover, since

$$A_{\Psi_A} = \frac{1}{\ell(A)} \sum_{k=1}^{\ell(A)} \gamma^{-k}(A)$$

so that $\omega(A_{\Psi_A}) = \omega(A)$ for all $\omega \in \mathcal{S}_\gamma(\mathcal{A})$, Theorem 2.4 (a) implies the variational expression in (4) for any $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$. The Lipschitz inequality in (3) for every $A, B \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ is immediately seen from the formula (2.3). Hence p_φ uniquely extends to a Lipschitz continuous function on \mathcal{A}^{sa} , and the convexity of p_φ on \mathcal{A}^{sa} is obvious. To prove (4) for general $A \in \mathcal{A}^{\text{sa}}$ let $\{A_n\}$ be a sequence in $\mathcal{A}_{\text{loc}}^{\text{sa}}$ such that $\|A_n - A\| \rightarrow 0$. It is clear by convergence that $p_\varphi(A) \geq -\omega(A) - S_M(\omega, \varphi)$ for all $\omega \in \mathcal{S}_\gamma(\mathcal{A})$. Let ω_n be the maximizer of the right-hand side of (4) for A_n ; here it may be assumed that $\{\omega_n\}$ converges to $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ in the weak* topology. Then we get

$$p_\varphi(A) = \lim_{n \rightarrow \infty} \{-\omega_n(A_n) - S_M(\omega_n, \varphi)\} \leq \omega(A) - S_M(\omega, \varphi)$$

by Lemma 2.3 (the weak* lower semicontinuity), which proves (4). Finally, (5) follows from Lemma 2.3 and the duality theorem for conjugate functions [13, Proposition I.4.1]. \square

For each $A \in \mathcal{A}^{\text{sa}}$ we have the convex and continuous function $t \mapsto p_\varphi(tA)$ on \mathbb{R} by Corollary 2.5 (3). We now introduce the function

$$I_A(x) := \inf\{S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A}), \omega(A) = x\} \quad (x \in \mathbb{R}). \quad (2.4)$$

Obviously, $I_A(x) = +\infty$ for $x \notin [\lambda_{\min}(A), \lambda_{\max}(A)]$, where $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ are the minimum and the maximum of the spectrum of A . The next proposition says that $p_\varphi(tA)$ and $I_A(x)$ are the Legendre transforms of each other, which are the contractions of the expressions in the above (5) and (4) into the real line via $\omega \mapsto \omega(A)$.

Proposition 2.6. *For every $A \in \mathcal{A}^{\text{sa}}$,*

$$\begin{aligned} I_A(x) &= \sup\{-tx - p_\varphi(tA) : t \in \mathbb{R}\}, & x \in \mathbb{R}, \\ p_\varphi(tA) &= \max\{-tx - I_A(x) : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}, & t \in \mathbb{R}. \end{aligned}$$

Proof. We have

$$\begin{aligned} I_A(x) &= \min_{\omega \in \mathcal{S}_\gamma(\mathcal{A})} \sup_{t \in \mathbb{R}} \{t(-x + \omega(A)) + S_M(\omega, \varphi)\} \\ &= \sup_{t \in \mathbb{R}} \min_{\omega \in \mathcal{S}_\gamma(\mathcal{A})} \{t(-x + \omega(A)) + S_M(\omega, \varphi)\} \\ &= \sup_{t \in \mathbb{R}} \{-tx - p_\varphi(tA)\} \end{aligned}$$

by Corollary 2.5 (4). In the above, the second equality follows from Sion's minimax theorem [35] thanks to Lemma 2.3. (The elementary proof in [25] for real-valued functions can also work for functions with values in $(-\infty, +\infty]$.) The second formula follows from the first by duality. \square

Remark 2.7. An alternative notion of free energy density

$$\tilde{p}_\varphi(A) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \varphi \left(\exp \left(\sum_{k=0}^{n-1} \gamma^k(A) \right) \right) \quad (2.5)$$

was recently studied in [29, 26, 17] in relation with large deviation problems on the spin chain. The function $t \in \mathbb{R} \mapsto \tilde{p}_\varphi(tA)$ is the so-called logarithmic moment generating function [12] of a sequence of probability measures and existence of the limit guarantees large deviation upper bound to hold, while if the limit is even differentiable that provides full large deviation principle. The existence of the limit was proven for any $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ when φ is the unique Gibbs state of a translation-invariant interaction of finite range [26] and when φ is a finitely correlated state [17]. Differentiability was shown in [29] and [17] for certain special cases. The Golden-Thompson inequality shows that

$$p_\varphi(A) \leq \tilde{p}_\varphi(A) \quad (2.6)$$

holds for any $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$. For instance, for a product state $\varphi = \bigotimes_{\mathbb{Z}} \rho$ with $D(\rho) = e^{-H}$ and a one-site observable A , since $\tilde{p}_\varphi(A) = \log \text{Tr}(e^{-H} e^{-A})$ while $p_\varphi(A) = \log \text{Tr}(e^{-H-A})$, the equality $p_\varphi(A) = \tilde{p}_\varphi(A)$ occurs only when A commutes with H (see [16]). Although the Lipschitz continuity of \tilde{p}_φ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ and its variational expression as in the above (4) are impossible, it might be possible to get the variational expression as in (5) with \tilde{p}_φ in place of p_φ . This is equivalent to saying that p_φ on \mathcal{A}^{sa} is the lower semicontinuous convex envelope of \tilde{p}_φ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$, as will be shown in a special case in Section 4 (see Corollary 4.10).

Remark 2.8. An equivalent formulation of the celebrated conjecture due to Bessis, Moussa and Villani [9] (the so-called BMV-conjecture) is stated as follows [27]: If H_0 and H_1 are $N \times N$ Hermitian matrices with $H_1 \geq 0$, then there exists a positive measure μ on $[0, \infty)$ such that

$$\text{Tr } e^{H_0 - tH_1} = \int_0^\infty e^{-ts} d\mu(s), \quad t > 0;$$

or equivalently, the function $\text{Tr } e^{H_0 - tH_1}$ on $t > 0$ is completely monotone. Now if the BMV-conjecture held true with

$$H_0 := \log D(\varphi_n), \quad H_1 := \frac{1}{n} \sum_{\Lambda+k \in [1, n]} \gamma^k(A),$$

where $A \in \mathcal{A}_\Lambda^{\text{sa}}$ with a finite $\Lambda \subset \mathbb{Z}$, we would have a probability measure μ_n supported in $[\lambda_{\min}(A), \lambda_{\max}(A)]$ such that

$$\text{Tr } \exp \left(\log D(\varphi_n) - \sum_{\Lambda+k \in [1, n]} \gamma^k(tA) \right) = \int_{-\infty}^\infty e^{-nts} d\mu_n(s), \quad t \in \mathbb{R}.$$

(The restriction on the support of μ_n easily follows from the Paley-Wiener theorem.) In this situation, the free energy density $p_\varphi(tA)$ is the logarithmic moment generating function of the sequence of measures (μ_n) , and Corollary 2.5 and Proposition 2.6 combined with the Gärtner-Ellis theorem [12, Theorem 2.3.6] yield that (μ_n) satisfies the large deviation principle with the good rate function $I_A(x)$ given in (2.4).

3 Perturbation of Gibbs states

When the reference state φ is a product state and A is a one-site observable, the variational expression of functional free energy density

$$\begin{aligned} \lim_{n \rightarrow \infty} \frac{1}{n} \log \operatorname{Tr} \exp(\log D(\varphi_n) - n f(s_n(A))) \\ = \sup_{\omega} \left\{ - \lim_{n \rightarrow \infty} \omega(f(s_n(A))) - S_M(\omega, \varphi) \right\} \end{aligned}$$

was obtained in [33], where ω runs over the symmetric (or permutation-invariant) states. A comprehensive exposition on the subject is also found in [31, §13], which contains a generalization of the above expression though φ is still a product state. In this section we consider the case when the reference state φ is the Gibbs state for a translation-invariant interaction Φ of finite range.

Let $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$. We may assume without loss of generality that $A \in \mathcal{A}_{[1, \ell(A)]}^{\text{sa}}$ with some $\ell(A) \in \mathbb{N}$, and set

$$s_n(A) := \frac{1}{n} \sum_{k=0}^{n-\ell(A)} \gamma^k(A) \in \mathcal{A}_{[1, n]}.$$

Given A and a continuous function $f : [\lambda_{\min}(A), \lambda_{\max}(A)] \rightarrow \mathbb{R}$ the *functional free energy density* is defined as the limit

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log Z_{\varphi}(n, A, f)$$

for

$$Z_{\varphi}(n, A, f) := \operatorname{Tr} \exp(\log D(\varphi_n) - n f(s_n(A)))$$

as $n \rightarrow \infty$. We will show the existence of the limit in Theorem 3.4.

The extreme boundary $\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})$ of the set $\mathcal{S}_{\gamma}(\mathcal{A})$ consists of the ergodic states. It is known that $\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})$ is a G_{δ} -subset of $\mathcal{S}_{\gamma}(\mathcal{A})$ (see [34, Proposition 1.3]). Since (\mathcal{A}, γ) is asymptotically Abelian in the norm sense, $\mathcal{S}_{\gamma}(\mathcal{A})$ is a so-called Choquet simplex (see [10, Corollary 4.3.11]) so that each $\omega \in \mathcal{S}_{\gamma}(\mathcal{A})$ has a unique extremal decomposition

$$\omega = \int_{\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})} \psi d\nu_{\omega}(\psi)$$

with a probability Borel measure ν_{ω} on $\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})$ (see [34, p. 66], [10, Theorem 4.1.15]).

Lemma 3.1. *For every continuous $f : [\lambda_{\min}(A), \lambda_{\max}(A)] \rightarrow \mathbb{R}$ and for every $\omega \in \mathcal{S}_{\gamma}(\mathcal{A})$ the limit*

$$E_{A, f}(\omega) := \lim_{n \rightarrow \infty} \omega(f(s_n(A)))$$

exists and

$$E_{A, f}(\omega) = \int_{\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})} f(\psi(A)) d\nu_{\omega}(\psi)$$

for the extremal decomposition $\omega = \int_{\operatorname{ex} \mathcal{S}_{\gamma}(\mathcal{A})} \psi d\nu_{\omega}(\psi)$.

Proof. The first assertion is contained in [31, Proposition 13.2]. However, we use a different method to prove the two statements together.

First let $\psi \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})$ and $(\pi_\psi, \mathcal{H}_\psi, U_\psi, \Omega_\psi)$ be the GNS construction associated with ψ , i.e., π_ψ is a representation of \mathcal{A} on \mathcal{H}_ψ with a cyclic vector Ω_ψ and U_ψ is a unitary on \mathcal{H}_ψ such that $\psi(A) = \langle \pi_\psi(A)\Omega_\psi, \Omega_\psi \rangle$ and $\pi_\psi(\gamma(A)) = U_\psi \pi_\psi(A) U_\psi^*$ for all $A \in \mathcal{A}$. Thanks to the asymptotic Abelianness, the extremality of ψ means (see [10, Theorem 4.3.17]) that the set of U_ψ -invariant vectors in \mathcal{H}_ψ is the one-dimensional subspace $\mathbb{C}\Omega_\psi$. Hence the mean ergodic theorem implies that

$$\pi_\psi(s_n(A))\Omega_\psi = \frac{1}{n} \sum_{k=0}^{n-\ell(A)} U_\psi^k \pi_\psi(A)\Omega_\psi$$

converges in norm to $\psi(A)\Omega_\psi$ as $n \rightarrow \infty$. The case $f(x) = x^m$ easily follows from this, and by approximating f by polynomials, we get

$$\lim_{n \rightarrow \infty} \|\pi_\psi(f(s_n(A)))\Omega_\psi - f(\psi(A))\Omega_\psi\| = 0$$

so that

$$\lim_{n \rightarrow \infty} \psi(f(s_n(A))) = f(\psi(A)).$$

Finally, for a general $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ with the extremal decomposition $\omega = \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} \psi \, d\nu_\omega(\psi)$, the Lebesgue convergence theorem gives

$$\lim_{n \rightarrow \infty} \omega(f(s_n(A))) = \lim_{n \rightarrow \infty} \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} \psi(f(s_n(A))) \, d\nu_\omega(\psi) = \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} f(\psi(A)) \, d\nu_\omega(\psi),$$

as required. \square

In the following proofs we will often use a state perturbation technique. For the convenience of the reader, we here summarize some basic properties of state perturbation restricted to the simple case of matrix algebras. See [11, 31] for the general theory of the subject matter. Let ρ be a faithful state of $\mathcal{B} := M_N(\mathbb{C})$ with density matrix e^{-H} . For each $h \in \mathcal{B}^{\text{sa}}$ define the perturbed functional ρ^h by

$$\rho^h(A) := \text{Tr } e^{-H-h} A \quad (A \in \mathcal{B})$$

and the normalized version

$$[\rho^h](A) := \frac{\rho^h(A)}{\rho^h(\mathbf{1})} = \frac{\text{Tr } e^{-H-h} A}{\text{Tr } e^{-H-h}} \quad (A \in \mathcal{B}).$$

The state $[\rho^h]$ is characterized as the unique minimizer of the functional

$$\omega \mapsto S(\omega, \rho) + \omega(h)$$

on the states of \mathcal{B} . It is plain to see the chain rule: $[[\rho^h]^k] = [\rho^{h+k}]$ for all $h, k \in \mathcal{B}^{\text{sa}}$. For each state ω of \mathcal{B} , from the equality

$$S(\omega, [\rho^h]) = S(\omega, \rho) + \omega(h) + \log \rho^h(\mathbf{1})$$

and the Golden-Thompson inequality $\rho^h(\mathbf{1}) \leq \rho(e^{-h})$, the following are readily seen:

$$\log \rho^h(\mathbf{1}) \geq -\omega(h) - S(\omega, \rho), \quad (3.1)$$

$$|S(\omega, \rho) - S(\omega, [\rho^h])| \leq 2\|h\|. \quad (3.2)$$

Lemma 3.2. *For every continuous $f : [\lambda_{\min}(A), \lambda_{\max}(A)] \rightarrow \mathbb{R}$ and for every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,*

$$\liminf_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) \geq \sup\{-E_{A,f}(\omega) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}$$

holds.

Proof. For $n \in \mathbb{N}$ write $h_n := nf(s_n(A))$ for simplicity. The perturbed functional $\varphi_n^{h_n}$ of φ_n on $\mathcal{A}_{[1,n]}$ has the density $\exp(\log D(\varphi_n) - h_n)$ and so $Z_\varphi(n, A, f) = \varphi_n^{h_n}(\mathbf{1})$. Hence it follows from (3.1) that

$$\log Z_\varphi(n, A, f) \geq -\omega_n(h_n) - S(\omega_n, \varphi_n), \quad \omega \in \mathcal{S}_\gamma(\mathcal{A}).$$

By Lemma 3.1 and (2.1) we have

$$\liminf_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) \geq -E_{A,f}(\omega) - S_M(\omega, \varphi)$$

for all $\omega \in \mathcal{S}_\gamma(\mathcal{A})$. □

Lemma 3.3. *For every continuous $f : [\lambda_{\min}(A), \lambda_{\max}(A)] \rightarrow \mathbb{R}$,*

$$\begin{aligned} & \sup\{-E_{A,f}(\omega) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\} \\ &= \sup\{-f(\psi(A)) - S_M(\psi, \varphi) : \psi \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})\} \\ &= \max\{-f(\omega(A)) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\} \\ &= \max\{-f(x) - I_A(x) : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}. \end{aligned}$$

Proof. For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ let $\omega = \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} \psi d\nu_\omega(\psi)$ be the extremal decomposition of ω . By Lemma 2.3 it follows from [34, Lemma 9.7] that

$$S_M(\omega, \varphi) = \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} S_M(\psi, \varphi) d\nu_\omega(\psi).$$

This together with Lemma 3.1 shows that

$$\begin{aligned} -E_{A,f}(\omega) - S_M(\omega, \varphi) &= \int_{\text{ex } \mathcal{S}_\gamma(\mathcal{A})} (-f(\psi(A)) - S_M(\psi, \varphi)) d\nu_\omega(\psi) \\ &\leq \sup\{-f(\psi(A)) - S_M(\psi, \varphi) : \psi \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})\}. \end{aligned}$$

Therefore,

$$\begin{aligned} & \sup\{-E_{A,f}(\omega) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\} \\ &\leq \sup\{-f(\psi(A)) - S_M(\psi, \varphi) : \psi \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})\}, \end{aligned}$$

and the converse inequality is obvious. Hence the first equality follows. The last equality immediately follows from the definition (2.4).

To prove the second equality, let $\tilde{\omega}$ be a maximizer of $\omega \mapsto -f(\omega(A)) - S_M(\omega, \varphi)$ on $\mathcal{S}_\gamma(\mathcal{A})$. For each $m \in \mathbb{N}$ with $m > \ell(A)$ we introduce a product state

$$\psi := \bigotimes_{\mathbb{Z}} \tilde{\omega}_m$$

of the re-localized spin chain $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$ and define $\bar{\psi} \in \mathcal{S}_\gamma(\mathcal{A})$ to be the average

$$\bar{\psi} := \frac{1}{m} \sum_{k=0}^{m-1} \psi \circ \gamma^k.$$

First we prove that $\bar{\psi}$ is γ -ergodic. For every $B_1, B_2 \in \mathcal{A}_{\text{loc}}$ choose an $i_0 \in \mathbb{N}$ such that $B_1, B_2 \in \mathcal{A}_{[-i_0m, (i_0-1)m]}$. Let $n \in \mathbb{N}$ be given so that $n = jm + r$ with $j \in \mathbb{N}$, $j > 2i_0$ and $0 \leq r < m$. When $i \geq 2i_0$, $1 \leq t \leq m$ and $0 \leq k \leq m-1$, we have

$$\psi(\gamma^k(B_1)\gamma^{k+im+t}(B_2)) = \psi(\gamma^k(B_1))\psi(\gamma^{k+im+t}(B_2)) = \psi(\gamma^k(B_1))\psi(\gamma^{k+t}(B_2)),$$

because $\gamma^k(B_1) \in \mathcal{A}_{(-\infty, i_0m]}$ and $\gamma^{k+im+t}(B_2) \in \mathcal{A}_{[(i-i_0)m+1, \infty)}$ with $i_0 \leq i - i_0$. Hence for every $i \geq 2i_0$ we get

$$\begin{aligned} \sum_{t=1}^m \bar{\psi}(B_1\gamma^{im+t}(B_2)) &= \frac{1}{m} \sum_{t=1}^m \sum_{k=0}^{m-1} \psi(\gamma^k(B_1))\psi(\gamma^{k+im+t}(B_2)) \\ &= \sum_{k=0}^{m-1} \psi(\gamma^k(B_1)) \left(\frac{1}{m} \sum_{t=1}^m \psi(\gamma^{k+t}(B_2)) \right) \\ &= \sum_{k=0}^{m-1} \psi(\gamma^k(B_1))\bar{\psi}(B_2) = m\bar{\psi}(B_1)\bar{\psi}(B_2). \end{aligned}$$

Therefore,

$$\begin{aligned} \frac{1}{n} \sum_{t=1}^n \bar{\psi}(B_1\gamma^t(B_2)) &= \frac{1}{n} \left(\sum_{t=1}^{2i_0m} + \sum_{t=jm+1}^{jm+r} \right) \bar{\psi}(B_1\gamma^t(B_2)) + \frac{1}{n} \sum_{i=2i_0}^{j-1} \sum_{t=1}^m \bar{\psi}(B_1\gamma^{im+t}(B_2)) \\ &= \frac{1}{n} \left(\sum_{t=1}^{2i_0m} + \sum_{t=jm+1}^{jm+r} \right) \bar{\psi}(B_1\gamma^t(B_2)) + \frac{(j-2i_0)m}{n} \bar{\psi}(B_1)\bar{\psi}(B_2), \end{aligned}$$

which obviously implies that

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{t=1}^n \bar{\psi}(B_1\gamma^t(B_2)) = \bar{\psi}(B_1)\bar{\psi}(B_2).$$

By [10, Theorems 4.3.17 and 4.3.22] this is equivalent to $\bar{\psi} \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})$. Furthermore, since

$$\bar{\psi}(A) = \frac{m - \ell(A) + 1}{m} \tilde{\omega}(A) + \frac{1}{m} \sum_{k=m-\ell(A)+1}^{m-1} \psi(\gamma^k(A)),$$

we get

$$|\bar{\psi}(A) - \tilde{\omega}(A)| \leq \frac{2\ell(A)\|A\|}{m}. \quad (3.3)$$

Now for m greater than both the range of Φ and $\ell(A)$, we set a product state

$$\phi^{(m)} := \bigotimes_{\mathbb{Z}} \varphi_m^G \quad (3.4)$$

of the re-localized $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$, where φ_m^G is the local Gibbs state of $\mathcal{A}_{[1, m]}$ for Φ . We also set

$$W := \sum \{ \Phi(X) : X \cap (-\infty, 0] \neq \emptyset, X \cap [1, \infty) \neq \emptyset \}, \quad (3.5)$$

$$K := \sum \{ \|\Phi(X)\| : X \cap (-\infty, 0] \neq \emptyset, X \cap [1, \infty) \neq \emptyset \} (\geq \|W\|). \quad (3.6)$$

For each $j \in \mathbb{N}$, since

$$H_{jm}(\Phi) = \sum_{i=0}^{j-1} \gamma^{im}(H_m(\Phi)) + \sum_{i=1}^{j-1} \gamma^{im}(W),$$

it is clear that $\phi^{(m)}|_{\mathcal{A}_{[1, jm]}} = \bigotimes_1^j \varphi_m^G$ is the perturbed state of φ_{jm}^G as follows:

$$\bigotimes_1^j \varphi_m^G = [(\varphi_{jm}^G)^{-W^{(m)}}], \quad (3.7)$$

where $W^{(m)} := \sum_{i=1}^{j-1} \gamma^{im}(W)$. Hence by Lemma 2.1 and (3.2) we get

$$\begin{aligned} S(\psi_{jm}, \varphi_{jm}) &\leq S(\psi_{jm}, \varphi_{jm}^G) + \log \lambda \\ &\leq S(\bigotimes_1^j \tilde{\omega}_m, \bigotimes_1^j \varphi_m^G) + 2(j-1)K + \log \lambda \\ &= jS(\tilde{\omega}_m, \varphi_m^G) + 2(j-1)K + \log \lambda \\ &\leq jS(\tilde{\omega}_m, \varphi_m) + 2(j-1)K + (j+1)\log \lambda. \end{aligned} \quad (3.8)$$

Since φ can be considered as the Gibbs state for an interaction of finite range in the re-localized $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$, Lemma 2.3 (the affine property) implies that

$$\begin{aligned} S_M(\bar{\psi}, \varphi) &= \frac{1}{m} \lim_{j \rightarrow \infty} \frac{1}{j} S(\bar{\psi}|_{\mathcal{A}_{[1, jm]}}, \varphi|_{\mathcal{A}_{[1, jm]}}) \\ &= \frac{1}{m^2} \sum_{k=0}^{m-1} \lim_{j \rightarrow \infty} \frac{1}{j} S(\psi \circ \gamma^k|_{\mathcal{A}_{[1, jm]}}, \varphi|_{\mathcal{A}_{[1, jm]}}) \\ &= \frac{1}{m} \lim_{j \rightarrow \infty} \frac{1}{j} S(\psi|_{\mathcal{A}_{[1, jm]}}, \varphi|_{\mathcal{A}_{[1, jm]}}) \end{aligned} \quad (3.9)$$

similarly to [31, (13.29)]. Therefore,

$$S_M(\bar{\psi}, \varphi) \leq \frac{1}{m} S(\tilde{\omega}_m, \varphi_m) + \frac{2K + \log \lambda}{m}. \quad (3.10)$$

From (3.3) and (3.10) together with (2.1), for any $\varepsilon > 0$ we have

$$-f(\bar{\psi}(A)) - S_M(\bar{\psi}, \varphi) \geq -f(\tilde{\omega}(A)) - S_M(\tilde{\omega}, \varphi) - \varepsilon,$$

whenever m is sufficiently large. With $\bar{\psi} \in \text{ex } \mathcal{S}_\gamma(\mathcal{A})$ this proves the second equality. \square

The next theorem showing the variational expression of the functional free energy density with respect to the state φ is a generalization of [33, Theorem 12] as well as [31, Theorem 13.11]. In fact, when φ is a product state $\bigotimes_{\mathbb{Z}} \rho$ and A is a one-site observable in \mathcal{A}_0 , one can easily see that

$$\begin{aligned} &\max \{ -f(\omega(A)) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A}) \} \\ &= \max \{ -f(\sigma(A)) - S(\sigma, \rho) : \sigma \text{ state of } \mathcal{A}_0 \} \end{aligned}$$

and

$$\begin{aligned} I_A(x) &= \min\{S(\sigma, \rho) : \sigma \text{ state of } \mathcal{A}_0, \sigma(A) = x\} \\ &= \sup\{-tx - \log \rho^{tA}(I) : t \in \mathbb{R}\} \end{aligned}$$

so that Theorem 3.4, together with Lemma 3.3, exactly becomes [33, Theorem 12]. A typical case is the quadratic function $f(x) = x^2$, which is familiar in quantum models of mean field type as remarked in [33] (also in Introduction).

The proof below is a modification of that of [31, Theorem 13.11]. Here it should be noted that the quantities $c(\varphi, nf(s_n(A)))$ in [31, §13] and $Z_\varphi(n, A, f)$ here are in the relation

$$c(\varphi, nf(s_n(A))) = -\log Z_\varphi(n, A, f)$$

as long as φ is a product state.

Theorem 3.4. *For every continuous $f : [\lambda_{\min}(A), \lambda_{\max}(A)] \rightarrow \mathbb{R}$ the limit*

$$p_\varphi(A, f) := \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f)$$

exists and

$$\begin{aligned} p_\varphi(A, f) &= \sup\{-E_{A,f}(\omega) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\} \\ &= \max\{-f(x) - I_A(x) : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}. \end{aligned}$$

Proof. By Lemmas 3.2 and 3.3 we only have to show that

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) \leq \sup\{-E_{A,f}(\omega) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}.$$

To prove this, we may assume by approximation that f is a polynomial. For each $m \in \mathbb{N}$ greater than both $\ell(A)$ and the range of Φ , let $\phi^{(m)} := \bigotimes_{\mathbb{Z}} \varphi_m^G$, a product state of the re-localized $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$ as in (3.4). Furthermore, we set

$$A^{(m)} := \frac{1}{m} \sum_{k=0}^{m-\ell(A)} \gamma^k(A) \in \mathcal{A}_{[1, m]}.$$

According to [33, Theorem 1] (or [31, Proposition 13.8]), for any $\varepsilon > 0$ there exists a symmetric (hence γ^m -invariant) state ψ of $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$ such that

$$\lim_{j \rightarrow \infty} \frac{1}{j} \log Z_{\phi^{(m)}}^{(m)}(j, A^{(m)}, mf) < -E_{A^{(m)}, mf}^{(m)}(\psi) - S_M^{(m)}(\psi, \phi^{(m)}) + \varepsilon, \quad (3.11)$$

where

$$\begin{aligned} Z_{\phi^{(m)}}^{(m)}(j, A^{(m)}, mf) &:= \text{Tr} \exp \left(\log \left(\bigotimes_1^j D(\varphi_m^G) \right) - jmf \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right), \\ E_{A^{(m)}, mf}^{(m)}(\psi) &:= \lim_{j \rightarrow \infty} \psi \left(mf \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right), \end{aligned}$$

$$S_M^{(m)}(\psi, \phi^{(m)}) := \lim_{j \rightarrow \infty} \frac{1}{j} S(\psi|_{\mathcal{A}_{[1, jm]}}, \phi^{(m)}|_{\mathcal{A}_{[1, jm]}}).$$

Then one can define an $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ by $\omega := \frac{1}{m} \sum_{k=0}^{m-1} \psi \circ \gamma^k$. Since we assumed that f is a polynomial, there is a constant $M > 0$ (depending on $\|A\|$) such that $\|f(B_1) - f(B_2)\| \leq M\|B_1 - B_2\|$ for all $B_1, B_2 \in \mathcal{A}^{\text{sa}}$ with $\|B_1\|, \|B_2\| \leq \|A\|$.

For each $n \in \mathbb{N}$ with $n \geq m$, write $n = jm + r$ where $j \in \mathbb{N}$ and $0 \leq r < m$. Since m is greater than the range of Φ , one can write

$$H_n(\Phi) = \sum_{i=0}^{j-1} \gamma^{im}(H_m(\Phi)) + \sum_{i=1}^{j-1} \gamma^{im}(W) + W_j,$$

where W is given in (3.5) and

$$W_j := \sum \{\Phi(X) : X \subset [1, n], X \cap [jm + 1, jm + r] \neq \emptyset\}.$$

We have by Lemma 2.1

$$\begin{aligned} \log D(\varphi_n) &\leq \log D(\varphi_n^G) + \log \lambda \\ &= - \sum_{i=0}^{j-1} \gamma^{im}(H_m(\Phi)) - \sum_{i=1}^{j-1} \gamma^{im}(W) - W_j \\ &\quad - \log \text{Tr} \exp \left(- \sum_{i=0}^{j-1} \gamma^{im}(H_m(\Phi)) - \sum_{i=1}^{j-1} \gamma^{im}(W) - W_j \right) + \log \lambda \\ &\leq \log(\otimes_1^j D(\varphi_m^G)) + 2jK + 2\|W_j\| + \log \lambda \end{aligned}$$

with K given in (3.6). Here it is clear that $\|W_j\| \leq mL$ with $L := \sum_{X \ni 0} \|\Phi(X)\|$. Furthermore, it is readily seen that

$$\left\| s_n(A) - \frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right\| \leq \left(\frac{2}{j} + \frac{\ell(A)}{m} \right) \|A\|$$

and hence

$$\left\| f(s_n(A)) - f \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right\| \leq \left(\frac{2}{j} + \frac{\ell(A)}{m} \right) M \|A\|. \quad (3.12)$$

Therefore,

$$\left\| nf(s_n(A)) - jmf \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right\| \leq m\|f\|_\infty + (2m + j\ell(A))M\|A\|,$$

where $\|f\|_\infty$ is the sup-norm of f on $[\lambda_{\min}(A), \lambda_{\max}(A)]$. From the above estimates we get

$$\begin{aligned} \frac{1}{n} \log Z_\varphi(n, A, f) &\leq \frac{1}{n} \log Z_{\phi^{(m)}}^{(m)}(j, A^{(m)}, mf) \\ &\quad + \frac{1}{n} \{ 2jK + 2mL + \log \lambda + m\|f\|_\infty + (2m + j\ell(A))M\|A\| \} \end{aligned}$$

so that

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) \leq \frac{1}{m} \lim_{j \rightarrow \infty} \frac{1}{j} \log Z_{\phi^{(m)}}^{(m)}(j, A^{(m)}, mf) + \frac{2K}{m} + \frac{\ell(A)M\|A\|}{m}. \quad (3.13)$$

Next, thanks to (3.12) we get

$$\begin{aligned} & \left| \omega(f(s_n(A))) - \psi \left(f \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right) \right| \\ & \leq \frac{1}{m} \sum_{k=0}^{m-1} \|f(\gamma^k(s_n(A))) - f(s_n(A))\| + \left\| f(s_n(A)) - f \left(\frac{1}{j} \sum_{i=0}^{j-1} \gamma^{im}(A^{(m)}) \right) \right\| \\ & \leq \frac{M}{m} \sum_{k=0}^{m-1} \|\gamma^k(s_n(A)) - s_n(A)\| + \left(\frac{2}{j} + \frac{\ell(A)}{m} \right) M\|A\| \\ & \leq \left(\frac{4}{j} + \frac{\ell(A)}{m} \right) M\|A\|. \end{aligned}$$

Therefore,

$$\left| E_{A,f}(\omega) - \frac{1}{m} E_{A^{(m)},mf}(\psi) \right| \leq \frac{\ell(A)M\|A\|}{m}. \quad (3.14)$$

Furthermore, we get

$$\begin{aligned} S(\psi_{jm}, \varphi_{jm}) & \leq S(\psi_{jm}, \varphi_{jm}^G) + \log \lambda \\ & \leq S(\psi|_{\mathcal{A}_{[1,jm]}}, \phi^{(m)}|_{\mathcal{A}_{[1,jm]}}) + 2(j-1)K + \log \lambda \end{aligned}$$

similarly to (3.8) using the state perturbation (3.7). Since

$$S_M(\omega, \varphi) = \frac{1}{m} \lim_{j \rightarrow \infty} \frac{1}{j} S(\psi|_{\mathcal{A}_{[1,jm]}}, \varphi|_{\mathcal{A}_{[1,jm]}})$$

in the same way as (3.9), it follows that

$$S_M(\omega, \varphi) \leq \frac{1}{m} S_M^{(m)}(\psi, \phi^{(m)}) + \frac{2K}{m}. \quad (3.15)$$

Inserting (3.13)–(3.15) into (3.11) gives

$$\limsup_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) \leq -E_{A,f}(\omega) - S_M(\omega, \varphi) + \frac{1}{m}(\varepsilon + 4K + 2\ell(A)M\|A\|),$$

implying the required inequality because m and ε are arbitrary. \square

The following is a straightforward consequence of Theorem 3.4.

Corollary 3.5. *For every continuous $f : \mathbb{R} \rightarrow \mathbb{R}$, the function $p_\varphi(\cdot, f)$ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ uniquely extends to a continuous function (denoted by the same $p_\varphi(\cdot, f)$) on \mathcal{A}^{sa} satisfying*

$$p_\varphi(A, f) = \max\{-f(x) - I_A(x) : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}$$

for all $A \in \mathcal{A}^{\text{sa}}$. Moreover, for every continuous $f, g : \mathbb{R} \rightarrow \mathbb{R}$ and every $A \in \mathcal{A}^{\text{sa}}$,

$$|p_\varphi(A, f) - p_\varphi(A, g)| \leq \max\{|f(x) - g(x)| : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}.$$

Remark 3.6. Suppose the “semi-classical” case where the observable $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ commutes with all $\Phi(X)$. Since $\alpha_t^\Phi(A) = A$ for all $t \in \mathbb{R}$, A belongs to the centralizer of φ , i.e., $\varphi(AB) = \varphi(BA)$ for all $B \in \mathcal{A}$. (To see this, apply [23, p. 617] in the GNS von Neumann algebra $\pi_\varphi(\mathcal{A})''$ having the modular automorphism group which extends α_t^Φ .) This implies that $s_n(A)$ commutes with $D(\varphi_n)$ for every $n \in \mathbb{N}$. As stated in Remark 2.8, $p_\varphi(tA)$ becomes the logarithmic moment generating function of (μ_n) satisfying the large deviation principle with the good rate function $I_A(x)$ in (2.4). For any continuous $f : \mathbb{R} \rightarrow \mathbb{R}$ we have

$$Z_\varphi(n, A, f) = \varphi_n(\exp(-nf(s_n(A)))) = \int_{\lambda_{\min}(A)}^{\lambda_{\max}(A)} e^{-nf(s)} d\mu_n(s).$$

Now Varadhan’s integral lemma [12, Theorem 4.3.1] can be applied to obtain

$$\lim_{n \rightarrow \infty} \frac{1}{n} \log Z_\varphi(n, A, f) = \max\{-f(x) - I_A(x) : x \in [\lambda_{\min}(A), \lambda_{\max}(A)]\}.$$

The exact large deviation principle is not formulated in our noncommutative setting as long as the BMV-conjecture remains unsolved (see Remark 2.8); nevertheless Varadhan’s formula is valid as stated in Theorem 3.4.

4 Perturbation of finitely correlated states

The notion of (C^*) -finitely correlated states was introduced by Fannes, Nachtergaele and Werner in [14]. Let \mathcal{B} be a finite-dimensional C^* -algebra, $\mathcal{E} : \mathcal{A}_0 \otimes \mathcal{B} \rightarrow \mathcal{B}$ ($\mathcal{A}_0 = M_d(\mathbb{C})$) a completely positive unital map and ρ a state of \mathcal{B} such that $\rho(\mathcal{E}(I \otimes b)) = \rho(b)$ for all $b \in \mathcal{B}$. For each $A \in \mathcal{A}_0$ define a map $\mathcal{E}_A : \mathcal{B} \rightarrow \mathcal{B}$ by $\mathcal{E}_A(b) := \mathcal{E}(A \otimes b)$, $b \in \mathcal{B}$. Then the *finitely correlated state* φ determined by the triple $(\mathcal{B}, \mathcal{E}, \rho)$ is the γ -invariant state of \mathcal{A} given by

$$\varphi(A_0 \otimes A_1 \otimes \cdots \otimes A_n) := \rho(\mathcal{E}_{A_0} \circ \mathcal{E}_{A_1} \circ \cdots \circ \mathcal{E}_{A_n}(\mathbf{1}_{\mathcal{B}})) \quad (A_i \in \mathcal{A}_i, \ 0 \leq i \leq n).$$

As was shown in the proof of [17, Proposition 4.4], a finitely correlated state has the following upper factorization property, which will be useful in our discussions below.

Lemma 4.1. *If φ is a finitely correlated state of \mathcal{A} , then there exists a constant $\alpha \geq 1$ such that*

$$\varphi \leq \alpha(\varphi|_{\mathcal{A}_{(-\infty, 0]}}) \otimes (\varphi|_{\mathcal{A}_{[1, \infty)}}).$$

The next proposition is a generalization of [31, Proposition 11.2].

Proposition 4.2. *Let φ be a finitely correlated state of \mathcal{A} . For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ the mean relative entropy*

$$S_M(\omega, \varphi) = \lim_{n \rightarrow \infty} \frac{1}{n} S(\omega_n, \varphi_n)$$

exists. Moreover, the function $\omega \in \mathcal{S}_\gamma(\mathcal{A}) \mapsto S_M(\omega, \varphi)$ is affine and weakly lower semicontinuous on $\mathcal{S}_\gamma(\mathcal{A})$.*

Proof. The proof of the first assertion is a slight modification of that of [20, Theorem 2.1] while it will be repeated below for the convenience of the remaining proof. For each $n, m \in \mathbb{N}$ with $n \geq m$, write $n = jm + r$ with $j \in \mathbb{N}$ and $0 \leq r < m$. Lemma 4.1 implies that

$$\varphi_n \leq \alpha^j \left(\bigotimes_{i=0}^{j-1} (\varphi|_{\mathcal{A}_{[im+1, (i+1)m]}}) \right) \otimes (\varphi|_{\mathcal{A}_{[jm+1, jm+r]}}). \quad (4.1)$$

Consider the product state $\phi^{(m)} := \bigotimes_{i \in \mathbb{Z}} \varphi_m$ of the re-localized spin chain $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$. For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ we have

$$S(\omega_n, \varphi_n) \geq S(\omega_{jm}, \varphi_{jm}) \geq S(\omega_{jm}, \bigotimes_1^j \varphi_m) - j \log \alpha \quad (4.2)$$

due to the monotonicity of relative entropy and (4.1). Dividing (4.2) by n and letting $n \rightarrow \infty$ with m fixed we get

$$\liminf_{n \rightarrow \infty} \frac{1}{n} S(\omega_n, \varphi_n) \geq \frac{1}{m} S_M^{(m)}(\omega, \phi^{(m)}) - \frac{\log \alpha}{m},$$

where $S_M^{(m)}(\omega, \phi^{(m)})$ denotes the mean relative entropy in the re-localized $\bigotimes_{i \in \mathbb{Z}} \mathcal{A}_{[im+1, (i+1)m]}$ as in (3.11). Since $S_M^{(m)}(\omega, \phi^{(m)}) \geq S(\omega_m, \varphi_m)$ by [18, (2.1)], we further get

$$\liminf_{n \rightarrow \infty} \frac{1}{n} S(\omega_n, \varphi_n) \geq \frac{1}{m} S(\omega_m, \varphi_m) - \frac{\log \alpha}{m}.$$

Since $m \in \mathbb{N}$ is arbitrary, this shows the existence of $S_M(\omega, \varphi)$ and the above inequalities become

$$S_M(\omega, \varphi) \geq \frac{1}{m} S(\omega_m, \varphi_m) - \frac{\log \alpha}{m}. \quad (4.3)$$

The affinity of $\omega \mapsto S_M(\omega, \varphi)$ is a consequence of the general property [31, Proposition 5.24]. Assume that $\omega, \omega^{(k)} \in \mathcal{S}_\gamma(\mathcal{A})$ and $\omega^{(k)} \rightarrow \omega$ weakly*. Then from (4.3) we have

$$\liminf_{k \rightarrow \infty} S_M(\omega^{(k)}, \varphi) \geq \frac{1}{m} \liminf_{k \rightarrow \infty} S(\omega_m^{(k)}, \varphi_m) - \frac{\log \alpha}{m} \geq \frac{1}{m} S(\omega_m, \varphi_m) - \frac{\log \alpha}{m}$$

thanks to the lower semicontinuity of relative entropy (in fact, $\omega \mapsto S(\omega_m, \varphi_m)$ is continuous due to finite dimensionality). Letting $m \rightarrow \infty$ shows the lower semicontinuity of $\omega \mapsto S_M(\omega, \varphi)$. \square

Next we show the existence of the free energy density with respect to a finitely correlated state φ . Since φ is not assumed to be locally faithful in the sense that $D(\varphi_n)$ is strictly positive for every $n \in \mathbb{N}$, we need to be careful in defining $\text{Tr} \exp(\log D(\varphi_n) - B)$ for $B \in \mathcal{A}_{[1, n]}^{\text{sa}}$. Let D be a nonzero positive semidefinite matrix and B a Hermitian matrix in $M_N(\mathbb{C})$. It is known [19, Lemma 4.1] that

$$\lim_{\varepsilon \searrow 0} e^{\log(D+\varepsilon I) - B} = P(e^{P(\log D)P - PBP})P,$$

where P is the support projection of D . Hence one can define $\text{Tr} e^{\log D - B}$ by

$$\text{Tr} e^{\log D - B} := \lim_{\varepsilon \searrow 0} \text{Tr} e^{\log(D+\varepsilon I) - B} = \text{Tr} P e^{P(\log D)P - PBP}. \quad (4.4)$$

Proposition 4.3. *Let φ be a finitely correlated state of \mathcal{A} . For every $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ so that $A \in \mathcal{A}_{\Lambda}^{\text{sa}}$ with a finite $\Lambda \subset \mathbb{Z}$, the free energy density*

$$p_{\varphi}(A) := \lim_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp \left(\log D(\varphi_n) - \sum_{\Lambda+k \subset [1,n]} \gamma^k(A) \right)$$

exists (independently of the choice of Λ). Moreover, p_{φ} is convex and Lipschitz continuous with $|p_{\varphi}(A) - p_{\varphi}(B)| \leq \|A - B\|$, and therefore it uniquely extends to a function on \mathcal{A}^{sa} with the same properties.

Proof. To prove the first assertion we may assume that $A \in \mathcal{A}_{[1, \ell(A)]}^{\text{sa}}$ with some $\ell(A) \in \mathbb{N}$. For each $n, m \in \mathbb{N}$ with $n \geq m > \ell(A)$, write $n = jm + r$ with $0 \leq r < m$. From (4.1) we get

$$D(\varphi_n) \leq \alpha^j \prod_{i=0}^{j-1} \gamma^{im}(D(\varphi_m))$$

with a constant $\alpha \geq 1$ independent of n, m . For any $\varepsilon > 0$ this implies that

$$D(\varphi_n) + \varepsilon^j I \leq \alpha^j \prod_{i=0}^{j-1} \gamma^{im}(D(\varphi_m) + \varepsilon I).$$

Furthermore, it is immediately seen that

$$\sum_{k=0}^{n-\ell(A)} \gamma^k(A) \geq \sum_{i=0}^{j-1} \gamma^{im} \left(\sum_{k=0}^{m-\ell(A)} \gamma^k(A) \right) - (j(\ell(A) - 1) + r) \|A\|.$$

Set $h_n := \sum_{k=0}^{n-\ell(A)} \gamma^k(A)$. From the above two inequalities we get

$$\begin{aligned} & \text{Tr} \exp(\log(D(\varphi_n) + \varepsilon^j I) - h_n) \\ & \leq \{ \text{Tr} \exp(\log(D(\varphi_m) + \varepsilon I) - h_m) \}^j \exp(j \log \alpha + (j(\ell(A) - 1) + r) \|A\|). \end{aligned}$$

In view of the definition (4.4), letting $\varepsilon \searrow 0$ gives

$$\begin{aligned} & \text{Tr} \exp(\log D(\varphi_n) - h_n) \\ & \leq \{ \text{Tr} \exp(\log D(\varphi_m) - h_m) \}^j \exp(j \log \alpha + (j(\ell(A) - 1) + r) \|A\|) \end{aligned}$$

so that

$$\begin{aligned} & \limsup_{n \rightarrow \infty} \frac{1}{n} \log \text{Tr} \exp(\log D(\varphi_n) - h_n) \\ & \leq \frac{1}{m} \log \text{Tr} \exp(\log D(\varphi_m) - h_m) + \frac{\log \alpha}{m} + \frac{\ell(A) - 1}{m} \|A\|. \end{aligned}$$

Since $m (> \ell(A))$ is arbitrary, this shows the existence of the limit $p_{\varphi}(A)$. It is obvious that $p_{\varphi}(A)$ is independent of the choice of Λ . It is also clear that $p_{\varphi}(A)$ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ is convex and satisfies $|p_{\varphi}(A) - p_{\varphi}(B)| \leq \|A - B\|$ for all $A, B \in \mathcal{A}_{\text{loc}}^{\text{sa}}$, from which the second part of the proposition follows. \square

Remark 4.4. The limit $\tilde{p}_\varphi(A)$ similar to $p_\varphi(A)$ was referred to in Remark 2.7 from the viewpoint of large deviations. In [17] the limit $\tilde{p}_\varphi(A)$ was shown to exist for any $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ when φ is a finitely correlated state (as well as when φ is a Gibbs state). The proof for $\tilde{p}_\varphi(A)$ is more involved than the above for $p_\varphi(A)$ and relies on the estimate in [26, Theorem 3.7] related to Gibbs state perturbation.

Once we had Propositions 4.2 and 4.3, it is natural to expect that $S_M(\omega, \varphi)$ and $p_\varphi(A)$ enjoy the same Legendre transform formulas as (4) and (5) of Corollary 2.5 in the Gibbs state case. But this is still unsolved while the following inequality is easy as Lemma 3.2. For the proof use [20, (4.2)] or [31, Proposition 1.11], the extended version of (3.1).

Proposition 4.5. *Let φ be a finitely correlated state of \mathcal{A} . For every $A \in \mathcal{A}^{\text{sa}}$,*

$$p_\varphi(A) \geq \max\{-\omega(A) - S_M(\omega, \varphi) : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}.$$

Remark 4.6. Suppose that φ satisfies the lower factorization property

$$\varphi \geq \beta(\varphi|_{\mathcal{A}_{(-\infty, 0]}}) \otimes (\varphi|_{\mathcal{A}_{[1, \infty)}})$$

for some $\beta > 0$ (the opposite version of Lemma 4.1). (In fact, it is enough to suppose a slightly weaker version of lower factorization as in [17, Definition 4.1].) Then all the results in Section 3 are true for φ . The proofs can be carried out similarly to those in Section 3; in fact, they are even easier without the state perturbation technique. However, the lower factorization property for finitely correlated states is quite strong; for example, one can easily see that a classical irreducible Markov chain has this property if and only if its transition stochastic matrix is strictly positive (i.e., all entries are strictly positive), which is stronger than the strong mixing property. More details are in [17].

In the rest of this section, we assume that φ is a γ -invariant *quantum Markov state* of Accardi and Frigerio type [3], and further assume that φ is locally faithful. According to [4, 30], there exists a conditional expectation E from $M_d(\mathbb{C}) \otimes M_d(\mathbb{C})$ into $M_d(\mathbb{C})$ such that $\varphi_0 \circ E(I \otimes A) = \varphi_0(A)$ for all $A \in M_d(\mathbb{C})$ and

$$\varphi(A_0 \otimes A_1 \otimes \cdots \otimes A_n) = \varphi_0(E(A_0 \otimes E(A_1 \otimes \cdots \otimes E(A_{n-1} \otimes A_n) \cdots)))$$

for all $A_0, A_1, \dots, A_n \in M_d(\mathbb{C})$, where $\varphi_0 := \varphi|_{\mathcal{A}_0}$. Set $\mathcal{B} := E(M_d(\mathbb{C}) \otimes M_d(\mathbb{C}))$, a subalgebra of $M_d(\mathbb{C})$, $\mathcal{E} := E|_{M_d(\mathbb{C}) \otimes \mathcal{B}}$ and $\rho := \varphi_0|_{\mathcal{B}}$. Then φ is a finitely correlated state with the triple $(\mathcal{B}, \mathcal{E}, \rho)$. Let q_1, \dots, q_k be the minimal central projections of \mathcal{B} ; then $\mathcal{B}q_i \cong M_{d_i}(\mathbb{C})$ and \mathcal{B} is decomposed as

$$\mathcal{B} = \bigoplus_{i=1}^k \mathcal{B}q_i = \bigoplus_{i=1}^k (M_{d_i}(\mathbb{C}) \otimes I_{m_i}),$$

where m_i is the multiplicity of $M_{d_i}(\mathbb{C})$ in $M_d(\mathbb{C})$. Let \mathcal{B}' be the relative commutant of \mathcal{B} in $M_d(\mathbb{C})$ so that $\mathcal{B}' = \bigoplus_{i=1}^k I_{d_i} \otimes M_{m_i}(\mathbb{C})$. For each $m, n \in \mathbb{Z}$, $m \leq n$, set

$$\tilde{\mathcal{A}}_{[m, n]} := \mathcal{B}' \otimes \mathcal{A}_{[m+1, n-1]} \otimes \mathcal{B} \quad (\subset \mathcal{A}_{[m, n]})$$

with convention $\tilde{\mathcal{A}}_{[n, n]} := \mathbb{C}I \subset \mathcal{A}_n$. Let $\mathcal{C} := \bigoplus_{i=1}^k M_{d_i}(\mathbb{C}) \otimes M_{m_i}(\mathbb{C}) \subset M_d(\mathbb{C})$ and $E_{\mathcal{C}}$ be the pinching $A \in M_d(\mathbb{C}) \mapsto \sum_{i=1}^k q_i A q_i \in \mathcal{C}$ (or the conditional expectation onto \mathcal{C} with respect to the trace). The following properties were shown in [4, 30]:

(i) There exist positive linear functionals ρ_{ij} on $M_{m_i}(\mathbb{C}) \otimes M_{d_j}(\mathbb{C})$, $1 \leq i, j \leq k$, such that

$$\mathcal{E} = \left(\bigoplus_{i,j=1}^k \text{id}_{M_{d_i}(\mathbb{C})} \otimes \rho_{ij} \right) \circ (E_{\mathcal{C}} \otimes \text{id}_{\mathcal{B}}).$$

(ii) Let T_{ij} be the density matrices of ρ_{ij} for $1 \leq i, j \leq k$. Then the density matrix of $\varphi|_{\tilde{\mathcal{A}}_{[m,n]}}$ is

$$\tilde{D}_{[m,n]} := \bigoplus_{i_m, i_{m+1}, \dots, i_n} \rho(q_{i_m}) T_{i_m i_{m+1}} \otimes T_{i_{m+1} i_{m+2}} \otimes \cdots \otimes T_{i_{n-1} i_n}. \quad (4.5)$$

The density matrices $\tilde{D}_{[m,n]}$ have a simple form of product type. Since T_{ij} is strictly positive in $M_{m_i}(\mathbb{C}) \otimes M_{d_j}(\mathbb{C})$ for each i, j due to the local faithfulness of φ , a γ -invariant nearest-neighbor interaction Φ can be defined by

$$\Phi([0, 1]) := - \sum_{i,j=1}^k \log T_{ij} \in \mathcal{B}' \otimes \mathcal{B} \subset \mathcal{A}_{[0,1]}, \quad \Phi([n, n+1]) := \gamma^n(\Phi([0, 1])).$$

Then the density of the local Gibbs state of $\mathcal{A}_{[m,n]}$ for Φ is

$$\bigoplus_{i_m, \dots, i_n} T_{i_m i_{m+1}} \otimes \cdots \otimes T_{i_{n-1} i_n},$$

and the automorphism group α_t^Φ is given by

$$\alpha_t^\Phi(A) = \lim_{m \rightarrow -\infty, n \rightarrow \infty} \tilde{D}_{[m,n]}^{-it} A \tilde{D}_{[m,n]}^{it} \quad (A \in \mathcal{A}). \quad (4.6)$$

Hence φ is the α^Φ -KMS state (or the Gibbs state for Φ) and so all the results in Sections 2 and 3 hold for φ . Below let us further investigate the relation between $p_\varphi(A)$ in (2.3) and $\tilde{p}_\varphi(A)$ in (2.5).

The centralizer of φ is given by

$$\mathcal{A}_\varphi := \{A \in \mathcal{A} : \varphi(AB) = \varphi(BA) \text{ for all } B \in \mathcal{A}\},$$

which is a γ -invariant C^* -subalgebra of \mathcal{A} . For each $m, n \in \mathbb{Z}$ with $m \leq n$, we also define

$$(\tilde{\mathcal{A}}_{[m,n]})_\varphi := \{A \in \tilde{\mathcal{A}}_{[m,n]} : \varphi(AB) = \varphi(BA) \text{ for all } B \in \tilde{\mathcal{A}}_{[m,n]}\}.$$

Lemma 4.7. *If $m' \leq m \leq n \leq n'$ in \mathbb{Z} , then $(\tilde{\mathcal{A}}_{[m,n]})_\varphi \subset (\tilde{\mathcal{A}}_{[m',n']})_\varphi \subset \mathcal{A}_\varphi$. Moreover, $\tilde{\mathcal{A}}_{\varphi, \text{loc}} := \bigcup_{n=1}^\infty (\tilde{\mathcal{A}}_{[-n,n]})_\varphi$ is a dense $*$ -subalgebra of \mathcal{A}_φ .*

Proof. Since $(\tilde{\mathcal{A}}_{[m,n]})_\varphi$ is the relative commutant of $\{\tilde{D}_{[m,n]}\}$ in $\tilde{\mathcal{A}}_{[m,n]}$, the first assertion is immediately seen from the form (4.5) of $\tilde{D}_{[m,n]}$. Furthermore, it is also obvious from (4.6) that $\alpha_t^\Phi(\tilde{\mathcal{A}}_{[m,n]}) = \tilde{\mathcal{A}}_{[m,n]}$, $t \in \mathbb{R}$, for any $m \leq n$. By [37] applied in the GNS von Neumann algebra $\pi_\varphi(\mathcal{A})''$ with the modular automorphism group extending α_t^Φ , there exists the conditional expectation $E_{[m,n]} : \mathcal{A} \rightarrow \tilde{\mathcal{A}}_{[m,n]}$ with $\varphi \circ E_{[m,n]} = \varphi$. Then it is clear that $\|E_{[m,n]}(A) - A\| \rightarrow 0$ as $m \rightarrow -\infty$ and $n \rightarrow \infty$ for any $A \in \mathcal{A}$. Now let $A \in \mathcal{A}_\varphi$. Since

$$\varphi(E_{[m,n]}(A)B) = \varphi(AB) = \varphi(BA) = \varphi(BE_{[m,n]}(A)), \quad B \in \tilde{\mathcal{A}}_{[m,n]},$$

we have $E_{[m,n]}(A) \in (\tilde{\mathcal{A}}_{[m,n]})_\varphi$ for any $m \leq n$, implying the latter assertion. \square

Lemma 4.8. For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,

$$S_M(\omega, \varphi) = \lim_{n \rightarrow \infty} \frac{1}{n} S(\omega|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi})$$

and hence $S_M(\omega, \varphi)$ is determined by $\omega|_{\mathcal{A}_\varphi}$. Moreover, if $\omega, \omega^{(i)} \in \mathcal{S}_\gamma(\mathcal{A})$, $i \in \mathbb{N}$, and $\omega^{(i)}|_{\mathcal{A}_\varphi} \rightarrow \omega|_{\mathcal{A}_\varphi}$ in the weak* topology, then

$$S_M(\omega, \varphi) \leq \liminf_{i \rightarrow \infty} S_M(\omega^{(i)}, \varphi).$$

Proof. The proof of the first assertion is essentially the same as that of [18, Theorem 2.1] as will be sketched below. Let $T_{ij} = \sum_{\ell=1}^{L_{ij}} \lambda_{ij\ell} e_{ij\ell}$ be the spectral decomposition of T_{ij} for $1 \leq i, j \leq k$, and Θ be the set of all (i, j, ℓ) with $1 \leq i, j \leq k$ and $1 \leq \ell \leq L_{ij}$. For each $n \in \mathbb{N}$ let K_n be the set of all tuples $(n_\theta)_{\theta \in \Theta}$ of nonnegative integers such that $\sum_{\theta \in \Theta} n_\theta = n-1$. For each $1 \leq i \leq k$ and $(n_\theta) \in K_n$ we denote by $I_{i, (n_\theta)}$ the set of all $(i_1, i_2, \dots, i_n; \ell_1, \ell_2, \dots, \ell_{n-1})$ such that $i_1 = i$ and $\#\{r \in [1, n-1] : (i_r, i_{r+1}, \ell_r) = \theta\} = n_\theta$ for all $\theta \in \Theta$, and define the projection $P_{i, (n_\theta)}$ in $\tilde{\mathcal{A}}_{[1,n]}$ and $\lambda_{i, (n_\theta)} \in \mathbb{R}$ by

$$P_{i, (n_\theta)} := \sum_{(i_1, \dots, i_n; \ell_1, \dots, \ell_{n-1}) \in I_{i, (n_\theta)}} e_{i_1 i_2 \ell_1} \otimes e_{i_2 i_3 \ell_2} \otimes \dots \otimes e_{i_{n-1} i_n \ell_{n-1}},$$

$$\lambda_{i, (n_\theta)} := \rho(q_i) \prod_{\theta \in \Theta} \lambda_\theta^{n_\theta} \quad \text{where} \quad \lambda_\theta := \lambda_{ij\ell} \quad \text{for} \quad \theta = (i, j, \ell).$$

Then $\sum_{i=1}^k \sum_{(n_\theta) \in K_n} P_{i, (n_\theta)} = I$ and $\tilde{D}_{[1,n]}$ is written as

$$\tilde{D}_{[1,n]} = \sum_{i=1}^k \sum_{(n_\theta) \in K_n} \lambda_{i, (n_\theta)} P_{i, (n_\theta)}.$$

Now, for each $\omega \in \mathcal{S}_\gamma(\mathcal{A})$, the proof of [18, Theorem 2.1] implies that

$$S(\omega_{n-2}, \varphi_{n-2}) \leq S(\omega|_{\tilde{\mathcal{A}}_{[1,n]}}, \varphi|_{\tilde{\mathcal{A}}_{[1,n]}}) \leq S(\omega|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}) + \log k + \log \#K_n$$

for every $n \geq 3$. Since $\#K_n \leq n^{\#\Theta}$, we get

$$S_M(\omega, \varphi) \leq \liminf_{n \rightarrow \infty} \frac{1}{n} S(\omega|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}),$$

which proves the first assertion.

Set $\gamma := 1/\min_{1 \leq i \leq k} \rho(q_i)$. For each $m, m' \in \mathbb{N}$, since it follows from (4.5) that

$$\varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi \otimes (\tilde{\mathcal{A}}_{[m+1, m+m']})_\varphi} \leq \gamma (\varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}) \otimes (\varphi|_{(\tilde{\mathcal{A}}_{[m+1, m+m']})_\varphi}),$$

we get

$$\begin{aligned} & S(\omega|_{(\tilde{\mathcal{A}}_{[1, m+m']})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1, m+m']})_\varphi}) \\ & \geq S(\omega|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi \otimes (\tilde{\mathcal{A}}_{[m+1, m+m']})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi \otimes (\tilde{\mathcal{A}}_{[m+1, m+m']})_\varphi}) - \log \gamma \\ & \geq S(\omega|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}) + S(\omega|_{(\tilde{\mathcal{A}}_{[1, m']})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1, m']})_\varphi}) - \log \gamma \end{aligned}$$

due to the monotonicity and the superadditivity of relative entropy [31, Corollary 5.21]. Let ω and $\omega^{(i)}$ be given as stated in the lemma. For any $m \in \mathbb{N}$ and $n = jm + r$ with $j \in \mathbb{N}$ and $0 \leq r < m$, the above inequality gives

$$S(\omega^{(i)}|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,n]})_\varphi}) \geq jS(\omega^{(i)}|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}) - j \log \gamma.$$

Dividing this by n and letting $n \rightarrow \infty$ with m fixed we get

$$S_M(\omega^{(i)}, \varphi) \geq \frac{1}{m}S(\omega^{(i)}|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}) - \frac{\log \gamma}{m}$$

and hence

$$\liminf_{i \rightarrow \infty} S_M(\omega^{(i)}, \varphi) \geq \frac{1}{m}S(\omega|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}, \varphi|_{(\tilde{\mathcal{A}}_{[1,m]})_\varphi}) - \frac{\log \gamma}{m}.$$

Letting $m \rightarrow \infty$ gives the latter assertion. \square

In addition to the variational expression in Corollary 2.5 (5) we have

Theorem 4.9. *For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$,*

$$\begin{aligned} S_M(\omega, \varphi) &= \sup\{-\omega(A) - p_\varphi(A) : A \in \mathcal{A}_\varphi^{\text{sa}}\} \\ &= \sup\{-\omega(A) - \tilde{p}_\varphi(A) : A \in \mathcal{A}_{\text{loc}}^{\text{sa}}\}, \end{aligned}$$

where $\tilde{p}_\varphi(A)$ is given in (2.5).

Proof. The proof of the first equality is a simple duality argument. Set $\Gamma := \{\omega|_{\mathcal{A}_\varphi^{\text{sa}}} : \omega \in \mathcal{S}_\gamma(\mathcal{A})\}$, which is a weakly* compact and convex subset of $(\mathcal{A}_\varphi^{\text{sa}})^*$, the dual Banach space of the real Banach space $\mathcal{A}_\varphi^{\text{sa}}$. From Lemma 4.8 one can define $F : (\mathcal{A}_\varphi^{\text{sa}})^* \rightarrow [0, +\infty]$ by

$$F(f) := \begin{cases} S_M(\omega, \varphi) & \text{if } f = \omega|_{\mathcal{A}_\varphi^{\text{sa}}} \text{ with some } \omega \in \mathcal{S}_\gamma(\mathcal{A}), \\ +\infty & \text{otherwise,} \end{cases}$$

which is affine and weakly* lower semicontinuous on $(\mathcal{A}_\varphi^{\text{sa}})^*$ by Proposition 4.2 and Lemma 4.8. Corollary 2.5 (4) says that

$$p_\varphi(A) = \max\{-f(A) - F(f) : f \in (\mathcal{A}_\varphi^{\text{sa}})^*\}, \quad A \in \mathcal{A}_\varphi^{\text{sa}}.$$

Hence it follows by duality [13, Proposition I.4.1] that

$$F(f) = \sup\{-f(A) - p_\varphi(A) : A \in \mathcal{A}_\varphi^{\text{sa}}\}, \quad f \in (\mathcal{A}_\varphi^{\text{sa}})^*.$$

For every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ this means the first equality, which also gives

$$S_M(\omega, \varphi) = \sup\{-\omega(A) - p_\varphi(A) : A \in \tilde{\mathcal{A}}_{\varphi, \text{loc}}^{\text{sa}}\} \quad (4.7)$$

thanks to Lemma 4.7.

To prove the second equality, we show that $p_\varphi(A) = \tilde{p}_\varphi(A)$ for all $A \in \tilde{\mathcal{A}}_{\varphi, \text{loc}}^{\text{sa}}$. Thanks to Lemma 4.7 and the γ -invariance of p_φ and \tilde{p}_φ , we may assume that $A \in (\tilde{\mathcal{A}}_{[1,m]})_\varphi^{\text{sa}}$ for some $m \in \mathbb{N}$. For each $n \in \mathbb{N}$ and $0 \leq k \leq n - m$, we have $\gamma^k(A) \in (\tilde{\mathcal{A}}_{[1+k, m+k]})_\varphi \subset (\tilde{\mathcal{A}}_{[1,n]})_\varphi$ so that

$\exp(-\sum_{k=0}^{n-m} \gamma^k(A)) \in (\tilde{\mathcal{A}}_{[1,n]})_\varphi$. Furthermore, since $\tilde{\mathcal{A}}_{[1,n]} \subset \mathcal{A}_{[1,n]} \subset \tilde{\mathcal{A}}_{[0,n+1]}$, it is easy to see by Lemma 4.7 that $(\tilde{\mathcal{A}}_{[1,n]})_\varphi \subset (\mathcal{A}_{[1,n]})_\varphi$. Hence we get $\exp(-\sum_{k=0}^{n-m} \gamma^k(A)) \in (\mathcal{A}_{[1,n]})_\varphi$, which implies that $\exp(-\sum_{k=0}^{n-m} \gamma^k(A))$ commutes with the density $D(\varphi_n)$ so that

$$\varphi\left(\exp\left(-\sum_{k=0}^{n-m} \gamma^k(A)\right)\right) = \text{Tr} \exp\left(\log D(\varphi_n) - \sum_{k=0}^{n-m} \gamma^k(A)\right),$$

showing $p_\varphi(A) = \tilde{p}_\varphi(A)$ by definitions (2.3) and (2.5). From this and (4.7) we get

$$\begin{aligned} S_M(\omega, \varphi) &\leq \sup\{-\omega(A) - \tilde{p}_\varphi(A) : A \in \mathcal{A}_{\text{loc}}^{\text{sa}}\} \\ &\leq \sup\{-\omega(A) - p_\varphi(A) : A \in \mathcal{A}_{\text{loc}}^{\text{sa}}\} = S_M(\omega, \varphi) \end{aligned}$$

thanks to (2.6) and Corollary 2.5 (5), implying the second equality. \square

Corollary 4.10. *The function p_φ on \mathcal{A}^{sa} is the lower semicontinuous convex envelope of \tilde{p}_φ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$ in the sense that p_φ is the largest among lower semicontinuous and convex functions q on \mathcal{A}^{sa} satisfying $q \leq \tilde{p}_\varphi$ on $\mathcal{A}_{\text{loc}}^{\text{sa}}$.*

Proof. Let q be as stated in the corollary. Define $Q : (\mathcal{A}^{\text{sa}})^* \rightarrow (-\infty, +\infty]$ by

$$Q(f) := \sup\{-f(A) - q(A) : A \in \mathcal{A}^{\text{sa}}\} \quad (f \in (\mathcal{A}^{\text{sa}})^*).$$

Let us prove that

$$\begin{cases} Q(\omega) \geq S_M(\omega, \varphi) & \text{if } \omega \in \mathcal{S}_\gamma(\mathcal{A}), \\ Q(f) = +\infty & \text{if } f \in (\mathcal{A}^{\text{sa}})^* \setminus \mathcal{S}_\gamma(\mathcal{A}). \end{cases} \quad (4.8)$$

For $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ Theorem 4.9 gives

$$Q(\omega) \geq \sup\{-\omega(A) - \tilde{p}_\varphi(A) : A \in \mathcal{A}_{\text{loc}}^{\text{sa}}\} = S_M(\omega, \varphi).$$

For $f \in (\mathcal{A}^{\text{sa}})^* \setminus \mathcal{S}_\gamma(\mathcal{A})$ we may consider the following three cases:

- (a) $f(A) < 0$ for some positive $A \in \mathcal{A}_{\text{loc}}$,
- (b) $f(\mathbf{1}) \neq 1$,
- (c) $f(A) \neq f(\gamma(A))$ for some $A \in \mathcal{A}^{\text{sa}}$.

In case (a), since $q(\alpha A) \leq \tilde{p}_\varphi(\alpha A) \leq 0$ for $\alpha > 0$, we get $-f(\alpha A) - q(\alpha A) \geq -\alpha f(A) \rightarrow +\infty$ as $\alpha \rightarrow +\infty$. In case (b), since $q(\alpha \mathbf{1}) \leq \tilde{p}_\varphi(\alpha \mathbf{1}) = -\alpha$, we get $-f(\alpha \mathbf{1}) - q(\alpha \mathbf{1}) \geq -\alpha(f(\mathbf{1}) - 1) \rightarrow +\infty$ as $\alpha \rightarrow +\infty$ or $-\infty$ according as $f(\mathbf{1}) < 1$ or $f(\mathbf{1}) > 1$. Finally in case (c), since

$$q(\alpha(A - \gamma(A))) \leq \tilde{p}_\varphi(\alpha(A - \gamma(A))) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \varphi(e^{-\alpha(A - \gamma^n(A))}) = 0,$$

we get $-f(\alpha(A - \gamma(A))) - q(\alpha(A - \gamma(A))) \geq -\alpha f(A - \gamma(A)) \rightarrow +\infty$ as $\alpha \rightarrow +\infty$ or $-\infty$ according as $f(A) < f(\gamma(A))$ or $f(A) > f(\gamma(A))$. Hence (4.8) follows. By duality this implies that $q \leq p_\varphi$ on \mathcal{A}^{sa} . \square

In particular, when φ is the product state $\bigotimes_{\mathbb{Z}} \rho$ of a not necessarily faithful ρ , all the variational expressions in Corollary 2.5 and Theorem 4.9 are valid for φ , and so Corollary 4.10 holds for φ . Although we have no strong evidence, it might be conjectured that Corollary 4.10 is true generally for the Gibbs-KMS state φ treated in Sections 2 and 3.

5 Concluding remarks: guide to the case of arbitrary dimension

In this paper we confined ourselves to the one-dimensional spin chain case for the following reasons. First, our main motivation came from recent developments on large deviations in spin chains, where the differentiability of logarithmic moment generating functions is crucial. The corresponding functions in our setting are free energy density functions so that we wanted to provide their differentiability (see Theorem 2.4(c) and Corollary 2.5(2)), and the one-dimensionality is essential for this. Secondly, finitely correlated states treated in the latter half are defined only in a one-dimensional spin chain though some attempts to multi-dimensional extension were made for similar states of quantum Markov type (see [1, 2] for example). However, all the discussions (except the differentiability assertions) presented for a Gibbs state of one-dimension in Sections 2 and 3 can also work well in the setting of arbitrary dimension but in high temperature regime, which we outline below.

Consider a ν -dimensional spin chain $\mathcal{A} := \bigotimes_{k \in \mathbb{Z}^\nu} \mathcal{A}_k$, $\mathcal{A}_k = M_d(\mathbb{C})$, with the translation automorphism group γ_k , $k \in \mathbb{Z}^\nu$, and local algebras $\mathcal{A}_\Lambda := \bigotimes_{k \in \Lambda} \mathcal{A}_k$ for finite $\Lambda \subset \mathbb{Z}^\nu$. We denote by $\mathcal{B}(\mathcal{A})$ the set of all translation-invariant interactions Φ in \mathcal{A} of relatively short range, i.e., $|||\Psi||| := \sum_{X \ni 0} \|\Psi(X)\|/|X| < +\infty$, which is a real Banach space with the norm $|||\Psi|||$. Let $\Phi \in \mathcal{B}(\mathcal{A})$ and assume further that Φ is of finite body, i.e., $N(\Phi) := \sup\{|X| : \Phi(X) \neq 0\} < +\infty$ (weaker than the assumption of finite range). Then Φ is automatically of short range, i.e., $\|\Phi\| := \sum_{X \ni 0} \|\Phi(X)\| < +\infty$. It is well known [11, 22] that the one-parameter automorphism group α_t^Φ of \mathcal{A} is defined and all of the α^Φ -KMS condition, the Gibbs condition and the variational principle for states $\varphi \in \mathcal{S}_\gamma(\mathcal{A})$ are equivalent. The pressure (1.5) and the mean entropy (1.6), the main ingredients in the variational principle, can be defined in the van Hove limit of $\Lambda \rightarrow \infty$ (see [22, p.12] or [11, p.287]), but in our further discussions we may simply restrict to the parallelepipeds $\Lambda = \{(k_1, \dots, k_\nu) : 1 \leq k_i \leq n_i, 1 \leq i \leq \nu\}$ with $\Lambda \rightarrow \infty$ meaning $n_i \rightarrow \infty$ for $1 \leq i \leq \nu$.

A crucial point in the arbitrary dimensional setting is the following generalization of Lemma 2.1 given in [8] in high temperature regime with an inverse temperature β .

Lemma 5.1. *Let Φ be given as above and $r(\Phi) := \{2\|\Phi\|(N(\Phi) - 1)\}^{-1}$ (meant $+\infty$ if $N(\Phi) \leq 1$). Assume that $0 < \beta < 2r(\Phi)$ and $\varphi \in \mathcal{S}_\gamma(\mathcal{A})$ satisfies the Gibbs condition for $\beta\Phi$ (equivalently, the α^Φ -KMS condition at $-\beta$). Then there are constants λ_Λ such that*

$$\lambda_\Lambda^{-1} \varphi_\Lambda \leq \varphi_\Lambda^{\beta, G} \leq \lambda_\Lambda \varphi_\Lambda$$

and

$$\lim_{\Lambda \rightarrow \infty} \frac{\log \lambda_\Lambda}{|\Lambda|} = 0, \quad (5.1)$$

where $\varphi_\Lambda^{\beta, G}$ is the local Gibbs state of \mathcal{A}_Λ for $\beta\Phi$.

Even though a Gibbs state $\varphi \in \mathcal{S}_\gamma(\mathcal{A})$ for $\beta\Phi$ is not necessarily unique and constants λ_Λ are depending on Λ , property (5.1) is enough for us to show all the results in Section 2 (except the differentiability assertions mentioned above) in the same way under the situation where Φ is replaced by $\beta\Phi$ with β as in Lemma 5.1 and $\mathcal{B}_0(\mathcal{A})$ is replaced by $\mathcal{B}(\mathcal{A})$. In particular, it was formerly observed in [20, p.710–711] that for every $\omega \in \mathcal{S}_\gamma(\mathcal{A})$ the mean relative entropy

(2.1) exists and furthermore $S_M(\omega, \varphi) = 0$ if and only if ω is a Gibbs state for $\beta\Phi$ too. In fact, the latter assertion is immediate from the formula in Lemma 2.3 due to the equivalence of the Gibbs condition and the variational principle.

Next let $A \in \mathcal{A}_{\text{loc}}^{\text{sa}}$ so that we may assume that $A \in \mathcal{A}_{\Lambda_0}^{\text{sa}}$ with some parallelepiped $\Lambda_0 \subset \mathbb{Z}^\nu$ of the form mentioned above. Let f be a real continuous function on $[\lambda_{\min}(A), \lambda_{\max}(A)]$. For each parallelepiped Λ of the same form, we set

$$s_\Lambda(A) := \frac{1}{|\Lambda|} \sum_{\Lambda_0 + k \subset \Lambda} \gamma_k(A)$$

and

$$Z_\varphi(\Lambda, A, f) := \text{Tr} \exp(\log D(\varphi_\Lambda) - |\Lambda|f(s_\Lambda(A))) .$$

Then Lemmas 3.1 and 3.2 hold true in the same way as before. Moreover, the proof of Lemma 3.3 can easily be carried out in the present framework with slight modifications, for example, with replacing the uniform boundedness of surface energies by the asymptotic property

$$\frac{1}{|\Lambda|} \sum \{\|\Phi(X)\| : X \cap \Lambda \neq \emptyset, X \cap \Lambda^c \neq \emptyset\} \longrightarrow 0$$

as $\Lambda \rightarrow \infty$ of parallelepipeds Λ . This property holds in general for translation-invariant interactions of short range.

Finally, we can prove the existence of the functional free energy density

$$p_\varphi(A, f) := \lim_{\Lambda \rightarrow \infty} \frac{1}{|\Lambda|} \log Z_\varphi(\Lambda, A, f)$$

and its variational expressions in the same way as in Theorem 3.4. A key point in proving this is that the result for the product state case in [33] (or [31]) used in the proof of Theorem 3.4 can be applied as well since the dimension of the integer lattice is irrelevant in the situation of product/symmetric states. In this way, all the proofs in Section 3 of one dimension can easily be adapted to the present framework by using Lemma 5.1 and the property of short range for Φ , and the condition of finite range is not necessary.

Acknowledgements

The authors are grateful to an anonymous referee for his comments that are very helpful in improving the final version of the paper.

References

- [1] L. Accardi and F. Fidaleo, Quantum Markov fields, *Infin. Dimens. Anal. Quantum Probab. Relat. Top.* **6** (2003), 123–138.
- [2] L. Accardi and F. Fidaleo, Non-homogeneous quantum Markov states and quantum Markov fields, *J. Funct. Anal.* **200** (2003), 324–347.

- [3] L. Accardi and A. Frigerio, Markovian cocycles, *Proc. Roy. Irish Acad.* **83A**(2) (1983), 251–263.
- [4] L. Accardi and V. Liebscher, Markovian KMS-states for one-dimensional spin chains, *Infin. Dimens. Anal. Quantum Probab. Relat. Top.* **2** (1999), 645–661.
- [5] H. Araki, Gibbs States of a One Dimensional Quantum Lattice, *Comm. Math. Phys.* **14**, (1969), 120–157.
- [6] H. Araki, On uniqueness of KMS states of one-dimensional quantum lattice systems, *Comm. Math. Phys.* **44** (1975), 1–7.
- [7] H. Araki, Positive cone, Radon-Nikodym theorems, relative Hamiltonian and the Gibbs condition in statistical mechanics. An application of the Tomita-Takesaki theory, in *Proc. Internat. School of Physics (Enrico Fermi)*, 1976, pp. 64–100.
- [8] H. Araki and P. D. F. Ion, On the equivalence of KMS and Gibbs conditions for states of quantum lattice systems, *Comm. Math. Phys.* **35** (1974), 1–12.
- [9] D. Bessis, P. Moussa and M. Villani, Monotonic converging variational approximations to the functional integrals in quantum statistical mechanics, *J. Math. Phys.* **16** (1975), 2318–2325.
- [10] O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics 1*, 2nd edition, Springer-Verlag, 2002.
- [11] O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics 2*, 2nd edition, Springer-Verlag, 1997.
- [12] A. Dembo and O. Zeitouni, *Large Deviation Techniques and Applications*, Second edition, Springer, New York, 1998.
- [13] I. Ekeland and R. Temam, *Convex Analysis and Variational Problems*, Studies in Mathematics and its Applications, Vol. 1, North-Holland, Amsterdam-Oxford, 1976.
- [14] M. Fannes, B. Nachtergaele and R. F. Werner, Finitely correlated states on quantum spin chains, *Comm. Math. Phys.* **144** (1992), 443–490.
- [15] P. Hayden, R. Jozsa, D. Petz and A. Winter, Structure of states which satisfy strong subadditivity of quantum entropy with equality, *Comm. Math. Phys.* **246** (2004), 359–374.
- [16] F. Hiai, Equality cases in matrix norm inequalities of Golden-Thompson type, *Linear and Multilinear Algebra* **36** (1994), 239–249.
- [17] F. Hiai, M. Mosonyi and T. Ogawa, Large deviations and Chernoff bound for certain correlated states on the spin chain, preprint, 2007.
- [18] F. Hiai and D. Petz, The proper formula for relative entropy and its asymptotics in quantum probability, *Comm. Math. Phys.* **143** (1991), 99–114.
- [19] F. Hiai and D. Petz, The Golden-Thompson trace inequality is complemented, *Linear Algebra Appl.* **181** (1993), 153–185.

- [20] F. Hiai and D. Petz, Entropy densities for Gibbs states of quantum spin systems, *Rev. Math. Phys.* **5** (1993), 693–712.
- [21] F. Hiai and D. Petz, Entropy densities for algebraic states, *J. Funct. Anal.* **125** (1994), 287–308.
- [22] R. B. Israel, *Convexity in the Theory of Lattice Gases*, Princeton Univ. Press, Princeton, 1979.
- [23] R. V. Kadison and J. R. Ringrose, *Fundamentals of the Theory of Operator Algebras. Vol. II. Advanced Theory*, Amer. Math. Soc., Providence, RI, 1997.
- [24] A. Kishimoto, On uniqueness of KMS states of one-dimensional quantum lattice systems, *Comm. Math. Phys.* **47** (1976), 167–170.
- [25] H. Komiya, Elementary proof for Sion’s minimax theorem, *Kodai Math. J.* **11** (1988), 5–7.
- [26] M. Lenci and L. Rey-Bellet, Large deviations in quantum lattice systems: one-phase region, *J. Stat. Phys.* **119** (2005), 715–746.
- [27] E. H. Lieb and R. Seiringer, Equivalent forms of the Bessis-Moussa-Villani conjecture, *J. Stat. Phys.* **115** (2004), 185–190.
- [28] M. Mosonyi and D. Petz, Structure of sufficient quantum coarse-grainings, *Lett. Math. Phys.* **68** (2004), 19–30.
- [29] K. Netočný and F. Redig, Large deviations for quantum spin systems, *J. Stat. Phys.* **117** (2004), 521–547.
- [30] H. Ohno, Translation-Invariant Quantum Markov States, *Interdisciplinary Information Sciences* **10** (2004), 53–58.
- [31] M. Ohya and D. Petz, *Quantum Entropy and Its Use*, 2nd edition, Springer-Verlag, 2004.
- [32] D. Petz, First steps towards a Donsker and Varadhan theory in operator algebras, in *Quantum Probability and Applications IV*, Lecture Notes in Math., **1442**(1990), 311–319.
- [33] D. Petz, G. A. Raggio and A. Verbeure, Asymptotic of Varadhan-type and the Gibbs variational principle, *Comm. Math. Phys.* **121** (1989), 271–282.
- [34] R. R. Phelps, *Lectures on Choquet’s Theorem*, Van Nostrand, New York-Toronto-London-Melbourne, 1966.
- [35] M. Sion, On general minimax theorems, *Pacific J. Math.* **8** (1958), 171–176.
- [36] G. A. Raggio and R. F. Werner, Quantum statistical mechanics of general mean field systems, *Helvetica Phys. Acta* **62** (1989), 980–1003.
- [37] M. Takesaki, Conditional expectations in von Neumann algebras, *J. Funct. Anal.* **9** (1972), 306–321.